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             (FILE 'HOME' ENTERED AT 14:47:12 ON 21 NOV 2002)
             FILE 'REGISTRY' ENTERED AT 14:53:28 ON 21 NOV 2002
                        ACT TAT997P/A
                    102 SEA FILE=REGISTRY SSS FUL L1/102 gpds from hull file search
        Ll
        L2
                      1 S 157807-48-2
        L3
                        ACT TAT997I/A
                     47 SEA FILE=REGISTRY ABB=ON PLU=ON (210108-85-3/BI OR 210108-86- ← cpds
        L4
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             FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 21 NOV 2002
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                        E AYLWARD J/AU
             FILE 'REGISTRY' ENTERED AT 14:56:06 ON 21 NOV 2002
                    34 S 12 AND 2809.1.1/RID/34 apds from STR Seurch have this STE
        L5
                     68 S L2 NOT L5 - related cpis
        L6
             FILE 'HCAPLUS' ENTERED AT 14:56:30 ON 21 NOV 2002
                     28 S L5 28 Cites for L5 cpds
       L7
                                                                             2809.1.1 is me
                     29 S E15, E17, E20-23 - cites from inventor search 5 S L4 AND L8
        L8
                                                                              ring identifier for
        L9
                     23 S L7 NOT L9
        L10
               23 S L7 NOT L9
576393 S IMMUN? OR? CANCER? OR ?TUMOR? OR ?CARCINOGEN? OR NEOPLAS? OR This ring
        L11
             7 S L10 AND L11) 7 G +es
                    4 S L10 (L) (DMA OR THU OR PKT OR PAC OR BAC) /RL 4 Cites
       CL13
                                                                                    Thu = therapy
       L14
                     0 S L12 AND L13
       /L15
                     12 S L10 NOT L12-13
                                                                           PKT = pharmacokinoping
                3 & L15 AND ?INFLAMM? /3 Cites

9 & L15 NOT L16 / 9 cites -not related to then-BAC = Biol achvity
       L16
       /L17
61 a tes L18 STR 5 → 61 S L6
7 S L1
                     7 S L18(L) (DMA OR THU OR PKT OR PAC OR BAC)/RL
L19
L19
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Nelsted L20
                                                                           PAC = pharmaco -
                      4 S L19 AND (L11 OR ?INFLAMM?)
                     13 S L18 AND (L11 OR ?INFLAMM?)
                                                                            DMAZ
                     16 S L19-21 / 16 cites related to medical, ETZ
MANUEX 'ADISALERTS, ADISINSIGHT, ADISNEWS, BABS, BIOBUSINESS, BIOCOMMERCE, BIOSIS, BIOTECHNO, CANCERLIT, CAPLUS, CBNB, CEN, CIN, CONFSCI, DDFB, RIDDFU, DGENE, DIOGENES, DRUGB, DRUGLAUNCH, DRUGMONOG2, DRUGH, DRUGU,
             DRUGUPDATES, EMBAL, EMBASE, ESBIOBASE, ...' ENTERED AT 15:13:49 ON 21 NOV
             2002
                        SEA ?INGENOL? OR ?INGENAN? Index searching
                       3* FILE ADISALERTS
                       3* FILE ADISINSIGHT
                       1 *
                           FILE ADISNEWS
                      64*
                           FILE BABS
                       8* FILE BIOBUSINESS
                       0*
                          FILE BIOCOMMERCE
                     198
                           FILE BIOSIS
                           FILE BIOTECHNO
                      79
                           FILE CANCERLIT
                     267
                           FILE CAPLUS
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0* FILE CBNB

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              0*
                 FILE DRUGLAUNCH
              0*
                 FILE DRUGMONOG2
              0* FILE DRUGNL
             21* FILE DRUGU
              0* FILE DRUGUPDATES
              3* FILE EMBAL
            149
                 FILE EMBASE
             37* FILE ESBIOBASE
             8* FILE FEDRIP
              7*
                 FILE IFIPAT
              0*
                 FILE INVESTEXT
             12*
                 FILE IPA
             24* FILE JICST-EPLUS
             0* FILE KOSMET
             28* FILE LIFESCI
            99
                 FILE MEDLINE
            101
                 FILE NAPRALERT
             69* FILE PASCAL
              1
                 FILE PHAR
                 FILE PHARMAML
              2* FILE PROMT
                 FILE SCISEARCH
            181
             2* FILE SYNTHLINE
            315 FILE TOXCENTER
             44 FILE USPATFULL
               QUE ?INGENOL? OR ?INGENAN?
L23
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FILE 'TOXCENTER, CAPLUS, BIOSIS, SCISEARCH, EMBASE, NAPRALERT, MEDLINE, CANCERLIT, PASCAL, BABS' ENTERED AT 15:16:13 ON 21 NOV 2002

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L24 628 S EG1
L25 119 S EUPHORBIA FACTOR

L26 1 S L24 AND L25 / C.+e
L27 1522 S ?INGENOL? OR ?INGENAN?
L28 61 S L27 AND (ANGELAT? OR MONOANGELAT?)
L30 36 S L28 AND (IMMUN? OR CANCER? OR ANTICANCER? OR TUMOR? OR ANTITU
L31 0 S L30 AND (STIMULAT? (3A) (IMMUN? OR INFLAMM?))
L32 2 S L30 AND (TREAT? (5A) (TUMOR? OR CANCER?)) / 2 C+es
L33 34 S L30 NOT L32
L34 10 DUP REM L33 (24 DUPLICATES REMOVED) / L0 C+es
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=> d que 17 -I drew this broadly since Appl. was claiming a derivative Ĺĺ STR 1 Fusion is allowed NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM these 2 moieties can be joined DEFAULT ECLEVEL IS LIMITED GRAPH ATTRIBUTES: in any manner RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 21 STEREO ATTRIBUTES: NONE cp ds 102 SEA FILE=REGISTRY SSS FUL L1 102 L234 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND 2809.1.1/RID 34 Cpds W/ 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L5 28 Cites

L5 L7

TATE 09/888,997

\Rightarrow d ibib abs hitstr 112 l

[L12 ANSWER 1 OF 7 HCAPLUS / COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:20788 HCAPLUS

DOCUMENT NUMBER: 135:136837

TITLE: Dietary cancer risk from conditional cancerogens (

tumor promoters) in produce of livestock fed

on species of spurge (Euphorbiaceae) V. Skin irritant

and tumor-promoting diterpene ester toxins of the tigliane and ingenane type in the herbs Euphorbia nubica and Euphorbia helioscopia

contaminating fodder of livestock

AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Soliman,

Soliman M.; Gotta, Hubert; Sorg, Bernd; Hecker, Erich

CORPORATE SOURCE: Laboratory of Organic Chemistry, Tahrir Street,

National Research Center (NRC), Cairo, Dokki, Egypt

SOURCE: Journal of Cancer Research and Clinical Oncology

(2001), 127(1), 40-47 CODEN: JCROD7; ISSN: 0171-5216

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Irritant diterpene ester toxins were isolated from Euphorbia nubica and E. helioscopia, which are contaminants of the green fodder of livestock in Egypt. Fractionations of methanol exts. of aerial parts of both plants were monitored by the irritation unit on the mouse ear. Plant exts. were subjected to multiplicative distribution methods, yielding irritant hydrophilic fractions that were further purified by column chromatog. Final purifn. of the materials was achieved by TLC (silica gel) followed by HPLC, or by TLC alone. In this way, from E. nubica, five Euphorbia factors [Nu1 (I)-Nu5(V)] were isolated and characterized as short-chain polyfunctional diterpene esters of tigliane-type parent alcs. The two weak irritants I and III were triesters of 4-deoxy(4.alpha.)phorbol. II (R1 and R2 = COPh or COPr-i) was shown to be a triester of the stereoisomeric tigliane-type parent alc. 4-deoxyphorbol. Weak irritant IV probably is a positional isomer of II. V was characterized as a short-chain triester of 4,20-dideoxy-5.xi.-hydroxyphorbol. From E. helioscopia, six short- to medium-chain polyfunctional diterpene esters of the ingenane type, generally contg. unsatd. acids were obtained, i.e., four irritant esters of ingenol (Euphorbia factors H1, H2, H5, and H6) and two esters of 20-deoxyingenol (non-irritant Euphorbia substance HS4 (VI), and irritant Euphorbia factor H8). All irritant Euphorbia factors of the tigliane and ingenane diterpene ester type described in this investigation are considered to be more or less active tumor promoters, i.e., conditional (non-genotoxic) cancerogens. The Euphorbia factors assayed exhibited moderate (H1) to low (H8) relative tumor-promoting potency in comparison to the ingenane prototype DTE tumor promoter 3-TI.

TT 75567-37-2P, Euphorbia factor H1 75567-38-3P, Euphorbia factor H8 91413-73-9P, Euphorbia factor HS4
RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence);
BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(skin irritant and tumor-promoting diterpene ester toxins of tigliane and ingenane type in herbs Euphorbia nubica and Euphorbia helioscopia contaminating fodder of livestock)

RN 75567-37-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR) - la, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9-tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 91413-73-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR) - 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5a, 6-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9-tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

23

REFERENCE COUNT:

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 112 2

L12 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:4251 HCAPLUS

DOCUMENT NUMBER: 130:34353

TITLE: Dietary cancer risk conditional cancerogens in produce

of livestock fed on species of spurge (Euphorbiaceae).

Part 1. Skin irritant and tumor-promoting

ingenane-type diterpene esters in E. peplus, one of several herbaceous Euphorbia species contaminating fodder of livestock. [Erratum to document cited in

CA129:312034]

Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamby; AUTHOR(S):

Gotta, Hubert; Hecker, Erich

CORPORATE SOURCE: Laboratory Organic Chemistry, National Research

Center, Cairo, Egypt

Journal of Cancer Research and Clinical Oncology SOURCE:

(1998), 124(6), 351 CODEN: JCROD7; ISSN: 0171-5216

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal LANGUAGE: English

On page 135, in Table 2, the words "Low" in the last column should read

"Medium"; the complete column is reprinted.

75567-38-3P 82425-35-2P 88262-86-6P IT

91413-73-9P

RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP

(skin irritant and tumor-promoting ingenane-type diterpene esters in Euphorbia (Erratum))

RN75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 4, 7, 9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 82425-35-2 HCAPLUS

2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4-[(acetyloxy)methyl]-la,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 88262-86-6 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aR,6S,8aS,9R,10aR)-5-(acetyloxy)-4[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 91413-73-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR) - la, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5a, 6-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9-tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

TATE 09/888,997

=> d ibib abs hitstr 112 3

L12 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1998:577094 HCAPLUS

DOCUMENT NUMBER:

129:312034

TITLE:

Dietary cancer risk conditional cancerogens in produce of livestock fed on species of spurge (Euphorbiaceae).

Part 1. Skin irritant and tumor-promoting

ingenane-type diterpene esters in E. peplus, one of several herbaceous Euphorbia species contaminating

fodder of livestock

AUTHOR(S):

Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamdy; Gotta, Hubert; Hecker, Erich

CORPORATE SOURCE:

Laboratory Organic Chemistry, National Research

Center, Cairo, Egypt

SOURCE:

Journal of Cancer Research and Clinical Oncology

(1998), 124(3/4), 131-140

CODEN: JCROD7; ISSN: 0171-5216

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: LANGUAGE:

Journal English

Several herbaceous plants of the genus Euphorbia, widespread as weeds and contaminants of livestock fodder, were identified botanically and exts. of their aerial parts were tested for irritancy on the mouse ear. As compared to a std. probe of croton oil, the exts. of E. peplus, E. nubica, and E. helioscopia displayed irritancy. The most active ext. (that from E. peplus) was investigated by a fractionation procedure monitored by the mouse ear assay, and 5 molecularly uniform irritant E. factors Pel-Pe5 were identified as diterpene ester-type toxins. Together these factors comprise at least 11 ppm in the aerial parts. They were characterized individually to carry the diterpene parent alcs. ingenol, 20-deoxyingenol, and 20-deoxyingenol-6.alpha., 7.alpha.-epoxide. The irritancy of the aerial plant parts was caused mainly by the E. factors Pel and Pe2 together. Upon chronic administration of these irritants and hyperplasiogens as principal cancerogenic risk factors in the mouse skin initiation/promotion bioassay, Pel and Pe2 were established as tumor promoters.

75567-38-3P 82425-35-2P 88262-86-6P TT 91413-73-9P

RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(skin irritant and tumor-promoting ingenane-type diterpene esters in Euphorbia)

RN 75567-38-3 HCAPLUS

2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR) -1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 4, 7, 9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4[(acetyloxy)methyl]-la, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 7, 9tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 88262-86-6 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR)-5-(acetyloxy)-4-[(acetyloxy)methyl]-1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5a-hydroxy-1, 1, 7, 9-tetramethyl-1l-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 91413-73-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR) - la,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

=> d ibib abs hitstr 112 4

L12 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1998:577085 HCAPLUS

DOCUMENT NUMBER:

129:274976

TITLE:

Dietary cancer risk from conditional cancerogens in

produce of livestock fed on species of spurge

(Euphorbiahceae). Part 3. Milk of lactating goats fed on the skin irritant herb Euphorbia peplus is polluted

by tumor promoters of the ingenane diterpene

ester type

AUTHOR(S):

Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamdy;

Gminski, Richard; Hecker, Erich

CORPORATE SOURCE:

Laboratory Organic Chemistry, National Research

Center, Cairo, Egypt

SOURCE:

Journal of Cancer Research and Clinical Oncology

(1998), 124(6), 301-306

CODEN: JCROD7; ISSN: 0171-5216

PUBLISHER:

Springer-Verlag

DOCUMENT TYPE: LANGUAGE:

Journal English

AB Poisonous milk was investigated from lactating goats fed exptl. on aerial parts of the herb E. peplus. In milk exts., weakly irritant in the mouse-ear assay, diterpene ester toxins of the ingenane structural type (Euphorbia factor Pe 1, 2, 4) were detected by HPLC. The toxins were identical to diterpene esters in the aerial parts. Milk collected 15 days after cessation of the feeding was completely toxin free. The non-toxic parent alc. ingenol was also detected in the milk but not in the plant indicating a metabolic generation by the goats. The authors suggest a possible mechanism for the development of esophageal cancer in certain areas in Iran.

IT 75567-38-3 82425-35-2 91413-73-9

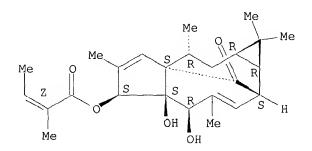
RL: POL (Pollutant); OCCU (Occurrence)

(milk of lactating goats fed on the skin irritant herb Euphorbia peplus is polluted by tumor promoters of the ingenane diterpene ester type)

RN 75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR) - 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 4, 7, 9-pentamethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.



RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4-

 $\label{localization} $$ [(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)$

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 91413-73-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR)1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5a, 6-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

=> d ibib abs hitstr 112 5

L12 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1984:507324 HCAPLUS

DOCUMENT NUMBER:

101:107324

TITLE:

On the active principles of the Euphorbiaceae, IX. Ingenane type diterpene esters from five Euphorbia

species

AUTHOR(S):

Gotta, H.; Adolf, W.; Opferkuch, H. J.; Hecker, E.

CORPORATE SOURCE:

Inst. Biochem., Dtsch. Krebsforschungszent.,

SOURCE:

Heidelberg, D-6900, Fed. Rep. Ger. Zeitschrift fuer Naturforschung, Teil B: Anorganische

Chemie, Organische Chemie (1984), 39B(5), 683-94

CODEN: ZNBAD2; ISSN: 0340-5087

DOCUMENT TYPE:

Journal English

LANGUAGE:

Investigation of E. antiquorum, E. helioscopia, E. palustris, E. peplus, and E. quadrialata for irritant and tumor-promoting constituents afforded several new ingenane diterpene esters derived from the parent

alcs. ingenol and 20-deoxyingenol and from the hitherto unknown 20-deoxy-16-hydroxyingenol and 20-deoxy-13,16-dihydroxyingenol. The irritant activities of the natural compatible are reported, together with

some aspects on structure activity relationships.

IT 75567-37-2 82425-35-2 88262-77-5

91413-73-9

RL: BIOL (Biological study)
 (from Euphorbia species)

RN 75567-37-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR) 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+): Double bond geometry as shown.

RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4[(acetyloxy)methyl]-la, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 7, 9tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 88262-77-5 HCAPLUS

RN 91413-73-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR) - 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5a, 6-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9-tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 75567-38-3P 88262-92-4P 91413-81-9P

RN 75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR) 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 4, 7, 9-pentamethyl-1l-oxo1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 88262-92-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, la,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-1-(hydroxymethyl)-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester,
[lR-[1.alpha.,la.beta.,2.alpha.,5.alpha.(Z),5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 91413-81-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, la,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1-(hydroxymethyl)-1,4,7,9-tetramethyl-ll-oxo-lH-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [lS-[l.alpha.,la.alpha.,2.beta.,5.beta.,5a.beta.,6.beta.(Z),8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)

=> d ibib abs hitstr 112 6

L12 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1984:12496 HCAPLUS

DOCUMENT NUMBER:

100:12496

TITLE:

3-O-Angeloylingenol, the toxic and skin irritant factor from latex of Euphorbia antiquorum L.

(Euphorbiaceae) and from a derived Thai purgative and

anthelimintic (vermifuge) drug

AUTHOR(S): CORPORATE SOURCE: Adolf, W.; Chanai, S.; Hecker, E. Inst. Biochem., Dtsch. Krebsforschungszent.,

Heidelberg, D-6900, Fed. Rep. Ger.

SOURCE:

Journal of the Science Society of Thailand (1983),

9(2), 81-8

CODEN: VKSTDB; ISSN: 0303-8122

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB From a latex of E. antiquorum, as well as from the purgative and anthelmintic (vermifuge) Thai drug yang Sa-Lad-Dai (dried, powd. latex), the highly skin irritant and toxic Euphorbia factor An1 3-O-angeloylingenol (I) [75567-37-2] was isolated by combination of countercurrent distributions and chromatog. Because of the acute toxicity of I and of the possible risk of cocarcinogenesis by tumor promotion, utilization of drugs made up from dried or fresh latex as practiced in Thailand in purgatives and vermifuges should be abandoned.

75567-37-2 ΤТ

RL: BIOL (Biological study)

(of Euphorbia antiquorum latex, skin irritation from)

Ι

RN75567-37-2 HCAPLUS

2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-CN 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

=> d ibib abs hitstr 112 7

L12 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2002 ACS 1983:12688 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

98:12688

On the active principles of the spurge family TITLE: (Euphorbiaceae). IV. Skin irritant and tumor

promoting diterpene esters from Euphorbia ingens E.

AUTHOR(S): Opferkuch, H. J.; Hecker, E.

Ι

CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent.,

Heidelberg, D-6900/1, Fed. Rep. Ger.

SOURCE: Journal of Cancer Research and Clinical Oncology

(1982), 103(3), 255-68 CODEN: JCROD7; ISSN: 0171-5216

DOCUMENT TYPE:

Journal English LANGUAGE:

GI

Me
$$CH_2R^5$$
 R^1O
 CH_2R^4
 CH_2OR^4

The irritant and tumor-promoting principles of the latex of AB Euphorbia ingens were isolated together with several nonirritant compds. The Euphorbia factor I1 [52557-26-3], I5 [52557-27-4], and I6 [52557-28-5] are esters of ingenane-type polyfunctional diterpene alcs. (I). Euphorbia factor II is characterized as the 3-hexadecanoate of I and Euphorbia factor I6 as the 3-deca-2.4.6-trienoic acid ester of I. Euphorbia factor I5 is the 16-angelate-3-deca-2.4.6-trienoate of 16-hydroxyingenol. Nonirritant diterpenes of the latex are I2 [39071-33-5], the ingenol-20-hexadecanoate - an isomer of Euphorbia factor I1 - and I4, the 3.7.12-triacetate-8-nicotinate of the macrocyclic lathyrane-type polyfunctional diterpene alc. ingol. The diterpene alcs. ingenol and 16-hydroxyingenol are inactive as irritants and tumor promoters of mouse skin. Compared to croton oil factor Al, the Euphorbia factor I1 exhibits .apprx.1/10 of the irritant and tumor -promoting activity in mouse skin. Il shows no reasonable tumorigenic activity. Compared with Il, Euphorbia factors I5 and I6 are more potent irritants and less potent tumor promoters.

ΙT 52557-27-4

RL: BIOL (Biological study)

(neoplasm promotion and skin irritation by)

52557-27-4 HCAPLUS RN

2,4,6-Decatrienoic acid, (1S,1aR,2S,5R,5aR,6S,8aS,9R,10aR)-CN 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-4-(hydroxymethyl)-1, 7, 9trimethyl-1-[[((2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-trimethyl-1-[((2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-trimethyl-1-[((2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-trimethyl-1-[((2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-trimethyl-1-[((2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethyl-1-oxo-1H-2,8a-trimethymethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester (9CI) (CA INDEX NAME)

PAGE 1-B

=> d ibib abs hitstr 113 1

L13 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:223682 HCAPLUS

DOCUMENT NUMBER: 129:321

TITLE: Comparative analysis of the vascular actions of

diterpenes isolated from Euphorbia canariensis

AUTHOR(S): Miranda, Francisco J.; Alabadi, Jose A.; Orti, Marta;

Centeno, Jose M.; Pinon, Marta; Yuste, Alberto; Sanz-Cervera, Juan F.; Marco, J. Alberto; Alborch,

Enrique

CORPORATE SOURCE: Department of Physiology, University of Valencia,

Valencia, E-46100, Spain

SOURCE: Journal of Pharmacy and Pharmacology (1998), 50(2),

237-241

CODEN: JPPMAB; ISSN: 0022-3573

PUBLISHER: Royal Pharmaceutical Society of Great Britain

DOCUMENT TYPE: Journal LANGUAGE: English

The effects of 2,3-diepiingol 7,12-diacetate-8-isobutyrate (I), ingenol-3-angelate-17-benzoate (II), ingenol-3-angelate-17-benzoate-20acetate (III) and 3,5,7,8,9,15-hexahydroxyjatropha-6(17),11-dien-14-one-5,8-bis(2-methylbutyrate)-7-(2-methylpropionate) (IV), isolated from E. canariensis, on the isometric tension developed by isolated rabbit basilar and carotid arteries were studied. Concn.-response curves to these compds. were obtained cumulatively in both arteries at resting tension and active tone (KCl, 50 mM). At resting tension a concn.-dependent contraction was induced by the four compds. In the basilar artery the order of potency was III = I > II = IV, without significant differences between Emax values. In the carotid artery the order of potency was III > II = I = IV and there were no significant differences between the Emax (max. effect) values of I-III, all of which were higher than that of IV. In pre-contracted basilar artery I-III induced concn.-dependent relaxation and IV was almost ineffective; the order of potency was III > II = I without significant differences between Emax values. In the carotid artery with active tone the four compds. induced further contractions; the order of potency was III > II = IV > I without significant differences between Emax values. These results show that the four diterpenes are potent active substances in rabbit basilar and carotid arteries and that there are regional differences between their action. All four compds. contract basilar and carotid arteries at resting tension. I-III relax pre-contracted basilar artery but not carotid artery.

IT 83983-93-1 192825-63-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(vascular actions of diterpenes isolated from Euphorbia canariensis)

RN 83983-93-1 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

192825-63-1 HCAPLUS RN

CN 2-Butenoic acid, 2-methyl-, (1R, laR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (22)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

=> d ind 113 1

ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS

CC 1-8 (Pharmacology)

ST Euphorbia diterpene vascular activity; ingenol analog Euphorbia vascular activity; jatrophane analog Euphorbia vascular activity; vasoconstrictor Euphorbia diterpene

ΙT Euphorbia canariensis

Vasoconstrictors

(vascular actions of diterpenes isolated from Euphorbia canariensis)

ΙΤ Diterpenes

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); BIOL (Biological study)

(vascular actions of diterpenes isolated from Euphorbia canariensis)

ΙT 83983-93-1 192825-63-1 207346-95-0 207346-96-1

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); BIOL (Biological study)

(vascular actions of diterpenes isolated from Euphorbia canariensis)

=> d ibib abs hitstr ind 113 2

L13 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1997:578751 HCAPLUS

DOCUMENT NUMBER: 127:257318

OCCUMENT NUMBER: 127.237316

TITLE: Analysis of the vascular effects of an ingenol

derivative isolated from Euphorbia canariensis

AUTHOR(S): Miranda, Francisco J.; Alabadi, Jose A.; Pinon, Marta; Orti, Marta; Centeno, Jose M.; Yuste, Alberto; Sanz-Cervera, Juan F.; Marco, J. Alberto; Alborch,

Enrique

CORPORATE SOURCE: Department of Physiology, University of Valencia,

Valencia, E-46100, Spain

SOURCE: Pharmaceutical Sciences (1997), 3(2), 113-116

CODEN: PHSCFB; ISSN: 1356-6881

PUBLISHER: Royal Pharmaceutical Society of Great Britain

DOCUMENT TYPE: Journal LANGUAGE: English

We have analyzed the effects of 3-O-[(Z)-2-methyl-2-butenoyl]-5,20-O-diacetyl-17-O-benzoyl-17-hydroxyingenol (MBDH), an ingenol deriv. isolated from Euphorbia canariensis, on isometric tension developed by isolated rabbit basilar and carotid arteries. MBDH concn.-response curves (10-8 - 3 .times. 10-5 M) were obtained cumulatively in precontracted (KCl, 50 mM) arteries. In basilar artery, MBDH induced a concn.-dependent relaxation that was not modified by incubation with NG-nitro-L-arginine (L-NOARG) (10-5 M) or indomethacin (10-5 M). In carotid artery, a slight relaxant response to MBDH was obsd. at higher concns., which turned into contraction in the presence of either indomethacin or L-NOARG. These results suggest that MBDH has a relaxant action on rabbit basilar and carotid arteries. Nitric oxide and prostacyclin mediate this relaxant action in carotid artery but do not participate in the response obtained in basilar artery.

IT 192825-66-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (vascular effects of an ingenol deriv. isolated from Euphorbia canariensis)

RN 192825-66-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 5,6-bis(acetyloxy)-[1-[(benzoyloxy)methyl]1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester,
[1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,
9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

CC 1-8 (Pharmacology)

ST Euphorbia ingenol deriv vasorelaxant prostacyclin NO

IT Euphorbia canariensis

Vasodilators

(vascular effects of an ingenol deriv. isolated from Euphorbia canariensis)

IT 192825-66-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (vascular effects of an ingenol deriv. isolated from Euphorbia canariensis)

IT 10102-43-9, Nitric oxide, biological studies 35121-78-9, Prostacyclin
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
 (Biological study); PROC (Process)
 (vascular effects of an ingenol deriv. isolated from Euphorbia
 canariensis)

=> d ibib abs hitstr ind 113 3

L13 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1989:454160 HCAPLUS

DOCUMENT NUMBER: 111:54160

TITLE: Toxic diterpenes from Euphorbia trigona (saiunkaku:

an indoor foliage plant in Japan) Tada, Masahiro; Seki, Hiromichi

AUTHOR(S): Tada, Masahiro; Seki, Hiromichi
CORPORATE SOURCE: Lab. Bio-Org. Chem., Tokyo Univ. Agric. Technol.,

Tokyo, 183, Japan

SOURCE: Agricultural and Biological Chemistry (1989), 53(2),

425-30

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE: Journal LANGUAGE: English

AB Three ingenol esters, displaying piscicidal activity, and an ingol ester were isolated from E. trigona. Their structures were unambiguously elucidated by means of IR, 1H- and 13C-NMR, and mass spectral data.

IT 82425-35-2 92998-75-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (from Euphorbia trigona, isolation and piscicidal activity of)

RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4[(acetyloxy)methyl]-la, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 7, 9tetramethyl-ll-oxo-lH-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 92998-75-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-1,4-bis[(acetyloxy)methyl]1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,
[1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.
beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

IT 121570-35-2

RL: BIOL (Biological study)
(from Euphorbia trigona, isolation and structure and piscicidal activity of)

RN 121570-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,4,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

CC 11-1 (Plant Biochemistry)
 Section cross-reference(s): 30

ST Euphorbia diterpene ingenol ingol ester piscicide

IT Euphorbia trigona

(ingenol and ingol esters from aerial parts of, isolation and structure and piscicidal activity of)

IT Piscicides

(ingenol esters from Euphorbia trigona as)

IT Diterpenes and Diterpenoids

RL: BIOL (Biological study)

(esters, from Euphorbia trigona, isolation and structure and piscicidal activity of)

IT 82425-35-2 92998-75-9

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); BIOL (Biological study)

(from Euphorbia trigona, isolation and piscicidal activity of)

IT 121570-35-2

RL: BIOL (Biological study)

(from Euphorbia trigona, isolation and structure and piscicidal

TATE 09/888,997

activity of) IT 121570-36-3

RL: BIOL (Biological study)
(from Euphorbia trigona, isolation and structure and plant growth inhibitory activity of)

=> d ibib abs hitstr ind 113 4

L13 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1985:557302 HCAPLUS

DOCUMENT NUMBER:

103:157302

TITLE:

Constituents of Egyptian Euphorbiaceae. Part 13. Biologically active diterpene esters from Euphorbia

peplus

AUTHOR (S):

Rizk, A. M.; Hammouda, F. M.; El-Missiry, M. M.;

Radwan, H. M.; Evans, F. J.

CORPORATE SOURCE:

Pharm. Sci. Lab., Natl. Res. Cent., Cairo, Egypt Phytochemistry (Elsevier) (1985), 24(7), 1605-6

CODEN: PYTCAS; ISSN: 0031-9422

DOCUMENT TYPE:

Journal

LANGUAGE:

SOURCE:

English

GI

- By means of partition and preparative TLC, 2 pro-inflammatory diterpene AΒ esters were isolated from E. peplus. These compds. were identified as 20-deoxyingenol 3-0-angelate, which exhibited an irritant dose (for 50% irritation) of 0.18 .mu.g on mouse skin, and the new ester ingenol 20-0-octanoate (I), which exhibited an irritant dose (for 50% irritation) of 1.0 .mu.g on mouse skin.
- 75567-38-3P TΤ

RL: PREP (Preparation)

(purifn. and inflammatory activity of, of Euphorbia peplus)

RN 75567-38-3 HCAPLUS

2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR) -CN la, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 4, 7, 9-pentamethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

- CC 11-1 (Plant Biochemistry)
 Section cross-reference(s): 4
- ST Euphorbia terpene deoxyingenolangelate ingenoloctanoate; irritant terpene Euphorbia
- IT Euphorbia peplus

(diterpene esters from)

- IT Esters, biological studies
 - RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
- (diterpenoid, inflammatory activity of, of Euphorbia peplus)
- IT Diterpenes and Diterpenoids
- RL: BAC (Biological activity or effector, except adverse); BSU
 - (Biological study, unclassified); BIOL (Biological study)
 - (esters, inflammatory activity of, of Euphorbia peplus)
- IT Skin, toxic chemical and physical damage
 - (irritation, from Euphorbia peplus diterpene esters)
- IT 30220-45-2P 54707-00-5P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
- IT **75567-38-3P** 98649-87-7P
 - RL: PREP (Preparation)
 - (purifn. and inflammatory activity of, of Euphorbia peplus)

=> d ibib abs hitstr ind 1

L16 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 2000:310802 HCAPLUS

DOCUMENT NUMBER:

133:86701

TITLE:

Diterpenoids from Euphorbia peplus

AUTHOR(S):

Hohmann, Judit; Evanics, Ferenc; Berta, Laszlo;

Bartok, Tibor

CORPORATE SOURCE:

Department of Pharmacognosy, Albert Szent-Gyorgyi

Medical University, Szeged, 6701, Hung. Planta Medica (2000), 66(3), 291-294

SOURCE:

CODEN: PLMEAA; ISSN: 0032-0943

PUBLISHER:

Georg Thieme Verlag

DOCUMENT TYPE: LANGUAGE:

Journal English

GI

O Me
OH Me
CH2 Me
PhCO2 H
OAc
i-PrCO2 OAc

AB From a pro-inflammatory active ext. of Euphorbia peplus, two new diterpene polyesters I and II based on the pepluane and jatrophane skeletons were isolated, together with four known ingenane and jatrophane diterpenes. The structures were detd. on the basis of extensive NMR studies. Ingenol 3-angelate, which was obtained for the first time from this plant, is an irritant toxin with high activity.

II

RN 75567-37-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

RN 75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR) - la, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 4, 7, 9-pentamethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 91413-73-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR)1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5a, 6-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

CC 11-1 (Plant Biochemistry)

TATE 09/888,997

Section cross-reference(s): 30 ST diterpenoid Euphorbia structure IT Euphorbia peplus New natural products (diterpenoids from Euphorbia peplus) ΙT RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (diterpenoids from Euphorbia peplus) ΙT Molecular structure, natural product (of diterpenoids from Euphorbia peplus) ΙT 75567-37-2 75567-38-3 91413-73-9 210108-85-3 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (diterpenoids from Euphorbia peplus) ΙT 280553-67**-**5P 280553-68-6P RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (diterpenoids from Euphorbia peplus) REFERENCE COUNT: THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS 7 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT ≈> d ibib abs hitstr ind 2

L16 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1989:109558 HCAPLUS

DOCUMENT NUMBER: 110:109558

TITLE: Irritancy of ingenol esters from Euphorbia kamerunica

AUTHOR(S): Abo, K. A.

CORPORATE SOURCE: Coll. Med., Univ. Ibadan, Nigeria SOURCE: Fitoterapia (1988), 59(3), 244-6 CODEN: FTRPAE; ISSN: 0367-326X

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

AB Six ingenol esters (I where R1 = H, dodecanoyl, decanoyl, Et, R2 = H, hexadienoyl, or octenoyl, and R3 = H or acetyl) showed irritant activity in the mouse ear assay. Monoesters were generally more potent than diesters. Monoesters exhibited chronic inflammation for .ltoreq.24 h. An ester function at C-3 or C-5 may be necessary for max. inflammatory response. A free C-20 primary etc. may be vital for max. activity and persistent inflammation.

IT 82425-35-2

RL: BIOL (Biological study)
(skin irritation from)

RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4[(acetyloxy)methyl]-la, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 7, 9tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

\approx d ibib abs hitstr ind 3

L16 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS 1982:452487 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

97:52487

TITLE:

Ingenol esters from the pro-inflammatory

fraction of Euphorbia kamerunica

AUTHOR (S):

Abo, Kio A.; Evans, Fred J.

CORPORATE SOURCE:

Dep. Pharmacogn., Sch. Pharm., London, WC1N 1AX, UK Phytochemistry (1982), 21(3), 725-6 CODEN: PYTCAS; ISSN: 0031-9422

SOURCE:

DOCUMENT TYPE:

Journal

LANGUAGE:

English

A series of unstable mono- and diesters of the tetracyclic diterpene irigenol were isolated from the proinflammatory ether-sol. fraction of the latex of E. kamerunica by column and thin-layer chromatog. The monoesters were identified by spectroscopic methods and hydrolysis reactions as the 3-decanoate, 3-dodecanoate, 5-hexadienoate, and 5-octenoate, and the diesters as 20-acetylingenol-3-octenoate and -3-angelate.

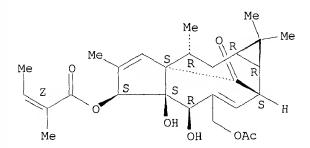
IT 82425-35-2

RL: BIOL (Biological study) (from Euphorbia kamerunica)

RN 82425-35-2 HCAPLUS

2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4-CN [(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.



CC11-1 (Plant Biochemistry)

Section cross-reference(s): 30

ST Euphorbia ingenol esters IT

Euphorbia kamerunica

(ingenol esters of)

IT Diterpenes and Diterpenoids

RL: BIOL (Biological study)

(ingenol esters, from Euphorbia kamerunica)

IT 30220-46-3D, esters 67021-88-9 82425-34-1 82425-35-2

82438-00-4 82438-02-6 82468-50-6

RL: BIOL (Biological study)

(from Euphorbia kamerunica)

TΤ 30220-45-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

0

TATE 09/888,997

=> d ibib abs hitstr ind 4
3 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):end

=> d ibib abs hitstr 1

L17 ANSWER 1 OF 9 HCAPLUS/ COPYRIGHT 2002 ACS ACCESSION NUMBER: 1998:671897 HCAPLUS

DOCUMENT NUMBER: 130:35626

TITLE: Ingenane and lathyrane diterpenes from the latex of

Euphorbia acrurensis

AUTHOR (S): Marco, J. Alberto; Sanz-Cervera, Juan F.; Ropero, F.

Javier; Checa, Javier; Fraga, B. Manuel

Departamento de Quimica Organica, Universidad de CORPORATE SOURCE:

Valencia, Valencia, E-46100, Spain

Phytochemistry (1998), 49(4), 1095-1099 CODEN: PYTCAS; ISSN: 0031-9422 SOURCE:

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

The latex of Euphorbia acrurensis yielded, in addn. to the widespread triterpenes euphol and euphorbol as the major components, two ingenol esters and nine lathyrane derivs. as minor components. All the lathyrane diterpenes were esters of ingol, and five of them were new. The structures were established with the aid of spectroscopic methods.

TΨ 88262-86-6 121570-35-2

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence) (from latex of Euphorbia acrurensis)

88262-86-6 HCAPLUS RN

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR) -5-(acetyloxy) -4-[(acetyloxy)methyl]-la,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 121570-35-2 HCAPLUS

2-Butenoic acid, 2-methyl-, (1R, 1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-1-CN [(acetyloxy)methyl]-1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 4, 7, 9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ind

L17 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2002 ACS

CC 11-1 (Plant Biochemistry)

Section cross-reference(s): 30

ST ingenane lathyrane diterpene Euphorbia

IT Diterpenes

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(from latex of Euphorbia acrurensis)

IT Euphorbia acrurensis

(ingenane and lathyrane diterpenes from latex of Euphorbia acrurensis)

IT Molecular structure, natural product

(of ingenol esters from Euphorbia acrurensis)

TT 514-47-6, Euphol 566-14-3, Euphorbol 58749-62-5 88262-86-6 89984-06-5 92910-93-5 92998-77-1 121570-35-2 RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

BIOL (Biological study); OCCU (Occurrence)

=> d ibib abs hitstr ind 2-9

L17 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1998:348270 HCAPLUS

DOCUMENT NUMBER: 129:109225

TITLE: Diterpenes from Euphorbia paralias

AUTHOR(S): Jakupovic, J.; Morgenstern, T.; Marco, J. A.;

Berendsohn, W.

CORPORATE SOURCE: Institute for Organic Chemistry, Technical University

of Berlin, Berlin, D-10623, Germany

SOURCE: Phytochemistry (1998), 47(8), 1611-1619

CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

- AB Chem. investigation of Euphorbia paralias from Spain afforded 13 diterpenes of different structural types, including one with a novel skeleton.
- IT 210046-66-5P 210047-56-6P
 RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)

(isolation and characterization of diterpenes from Euphorbia paralias)

Relative stereochemistry.

Double bond geometry as shown.

- RN 210047-56-6 HCAPLUS
- CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-11-oxo1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)-rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.

- CC 30-20 (Terpenes and Terpenoids) Section cross-reference(s): 11
- ST diterpene isolation Euphorbia paralias mol structure
- IT Euphorbia paralias
 - (isolation and characterization of diterpenes from Euphorbia paralias)
- IT Diterpenes

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)

(isolation and characterization of diterpenes from Euphorbia paralias)

IT Molecular structure, natural product

TΨ

SOURCE:

(of diterpenes)
205870-73-1P 205870-75-3P 210046-57-4P 210046-58-5P 210046-59-6P
210046-60-9P 210046-61-0P 210046-62-1P 210046-63-2P 210046-64-3P

210046-65-4P 210046-66-5P 210047-56-6P RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)

(isolation and characterization of diterpenes from Euphorbia paralias)

L17 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1998:348268 HCAPLUS

DOCUMENT NUMBER: 129:120130

TITLE: Diterpenes from Euphorbia segetalis

AUTHOR(S): Jakupovic, J.; Jeske, F.; Morgenstern, T.; Tsichritzis, F.; Marco, J. A.; Berendsohn, W.

CORPORATE SOURCE: Institute for Organic Chemistry, Technical University

of Berlin, Berlin, D-10623, Germany
Phytochemistry (1998) 47(8), 1583-16

Phytochemistry (1998), 47(8), 1583-1600 CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

AB Numerous new diterpenes including several with new skeletons have been obtained from Euphorbia segetalis.

IT 75567-38-3P 82425-35-2P 210158-15-9P

210158-16-0P 210158-17-1P

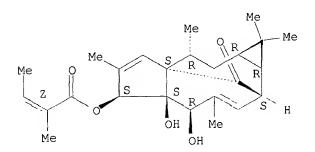
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)

(isolation and characterization of diterpenes from Euphorbia segetalis)

RN 75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR) 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 4, 7, 9-pentamethyl-1l-oxo1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.



RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (laR,2S,5R,5aS,6S,8aS,9R,10aR)-4[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 210158-15-9 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9trimethyl-1-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 210158-16-0 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R, 1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aS)-10a-(acetyloxy)-1-[(benzoyloxy)methyl]-1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 4, 7, 9-tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 210158-17-1 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)
1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,4,7,9-tetramethyl-1
[[((2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8a
methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CAINDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

CC 11-1 (Plant Biochemistry)
 Section cross-reference(s): 30

ST diterpene isolation Euphorbia segetalis

IT New natural products

(diterpenes from Euphorbia segetalis)

IT Euphorbia segetalis

(isolation and characterization of diterpenes from Euphorbia segetalis)

IT Diterpenes

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)

(isolation and characterization of diterpenes from Euphorbia segetalis)

IT Molecular structure, natural product

(of diterpenes from Euphorbia segetalis)

IT 54706-99-9P 64280-37-1P **75567-38-3P 82425-35-2P**

129134-90-3P 174974-43-7P, Terracinolide A 174974-44-8P, Terracinolide

B 190382-22-0P, Terracinolide C 190382-26-4P, Terracinolide E 210157-98-5P 210157-99-6P 210158-00-2P 210158-01-3P 210158-02-4P

210158-03-5P 210158-04-6P 210158-05-7P 210158-06-8P 210158-07-9P

210158-08-0P 210158-09-1P 210158-10-4P 210158-11-5P 210158-12-6P

210158-14-8P 210158-15-9P 210158-16-0P 210158-13-7P 210164-78-6P 210173-98-1P, Terracinolide H 210158-17-1P 210173-99-2P, Terracinolide I 210174-00-8P, 13.alpha.-210174-01-9P, 13.alpha.-Hydroxyterracinolide I Hydroxyterracinolide B RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)

(isolation and characterization of diterpenes from Euphorbia segetalis) 210158-18-2P 210158-19-3P TΤ

RL: SPN (Synthetic preparation); PREP (Preparation)

(isolation and characterization of diterpenes from Euphorbia segetalis)

ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2002 ACS 1997:380090 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 127:119554

Ingenane and lathyrane diterpenes from the latex of TITLE:

Euphorbia canariensis

AUTHOR(S): Marco, J. Alberto; Sanz-Cervera, Juan F.; Yuste,

Alberto

Dep. Quimica Organica, Univ. Valencia, Burjassot, CORPORATE SOURCE:

E-46100, Spain

Phytochemistry (1997), 45(3), 563-570 SOURCE:

CODEN: PYTCAS; ISSN: 0031-9422

PUBLISHER: Elsevier DOCUMENT TYPE: Journal English LANGUAGE:

GT

The latex of Euphorbia canariensis yielded, in addn. to five known ingenol AΒ esters, the ingenane derivs. ingenol 3-angelate 5,20-diacetate (I) and 5-deoxyingenol 3-angelate 20-acetate, and the lathyrane derivs. 2,3-diepiingol 7,12-diacetate 8-benzoate (II), 2,3-diepiingol 7,12-diacetate 8-isobutyrate and 2-epiingol 3,7,12-triacetate 8-benzoate.

The structures were established with the aid of spectroscopic methods, mainly NMR, and mol. mechanics calcns. They were also supported by the results of some chem. transformations.

TT 75567-37-2P 82425-35-2P 83966-48-7P 83983-93-1P 88262-75-3P 88262-86-6P 192825-63-1P 192825-64-2P

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis)

RN 75567-37-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-4[(acetyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (22)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 83966-48-7 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, [1-[(benzoyloxy)methyl]-1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a, 6-trihydroxy-1, 7, 9-trimethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha., 1a.beta., 2.alpha., 4(Z), 5.alpha., 5a.alpha., 6.alpha., 8a.beta., 9.beta., 10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 83983-93-1 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 88262-75-3 HCAPLUS

2-Butenoic acid, 2-methyl-, 1,4-bis[(acetyloxy)methyl]1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,
[lR-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

88262-86-6 HCAPLUS RN

2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR)-5-(acetyloxy)-4-[(acetyloxy)methyl]-la,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

192825-63-1 HCAPLUS RN

2-Butenoic acid, 2-methyl-, (1R, 1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4-[(acetyloxy)methyl]-1-[(benzoyloxy)methyl]-la,2,5,5a,6,9,10,10a-octahydro-CN 5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 192825-64-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 4-[(acetyloxy)methyl]-la,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,
[laR-[la.alpha.,2.beta.,5a.beta.,6.beta.(Z),8a.alpha.,9.alpha.,10a.alpha.]
]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

IT 192825-66-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and properties of)

RN 192825-66-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 5,6-bis(acetyloxy)-[1-[(benzoyloxy)methyl]la,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester,
[1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,
9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

CC 11-1 (Plant Biochemistry)

Section cross-reference(s): 30

ST ingenane lathyrane diterpene Euphorbia

IT Euphorbia canariensis

(ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis)

TATE 09/888,997

Diterpenes TΤ RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis) 75567-37-2P 82425-35-2P 83966-48-7P IT 83983-93-1P 88262-75-3P 88262-86-6P 192045-51-5P **192825-63-1P 192825-64-2P** 192825-65-3P 192865-19-3P RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (ingenane and lathyrane diterpenes from the latex of Euphorbia canariensis) 192825-66-4P 192865-20-6P 192865-24-0P IΤ RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and properties of) ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2002 ACS 1984:607619 HCAPLUS ACCESSION NUMBER: 101:207619 DOCUMENT NUMBER: Five ingol esters and a 17-hydroxyingenol ester from TITLE: the latex of Euphorbia kamerunica. Assignment of esters using carbon-13 NMR methods Connolly, Joseph D.; Fakunle, Christopher O.; Rycroft, AUTHOR(S): David S. Dep. Chem., Univ. Glasgow, Glasgow, G12 8QQ, UK CORPORATE SOURCE: Tetrahedron Letters (1984), 25(34), 3773-6 SOURCE: CODEN: TELEAY; ISSN: 0040-4039 DOCUMENT TYPE: Journal LANGUAGE: English The structures of 5 ingol esters and a 17-hydroxyingenol ester from the latex of E. kamerunica were detd. The 13C NMR spectra of these compds. have been assigned using 2D .delta.C/.beta.H correlations. The specific positions of attachment of esters have been assigned unambiguously using 13C NMR methods, including 2D long-range .delta.C/.delta.H correlations. The 5 ingol esters were 8-O-methylingol-3,12-diacetate-7-tiglate, 8-O-methylingol-3,12-diacetate-7-benzoate, ingol-3,8,12-triacetate-7tiglate, ingol-3,8,12-triacetate-7-angelate, and 8-0-methylingol-3,12diacetate-7-angelate. ΙT 92998-75-9 RL: BIOL (Biological study) (from latex of Euphorbia kamerunica) 92998-75-9 HCAPLUS 2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-1,4-bis[(acetyloxy)methyl]-CN 1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5a-hydroxy-1, 7, 9-trimethyl-11-oxo-1H-2, 8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, [1R-[1.alpha., la.beta., 2.alpha., 5.alpha., 5a.alpha., 6.alpha.(Z), 8a.beta., 9. beta., 10a.beta.]] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

CC 11-1 (Plant Biochemistry)

ST ingol ester Euphorbia latex; hydoxyingenol ester Euphorbia latex

IT Euphorbia kamerunica

(ingol esters from latex of)

IT Latex

(ingol esters from, Euphorbia kamerunica)

IT 89984-05-4 89984-06-5 90027-10-4 92910-93-5 **92998-75-9**

92998-77-1

RL: BIOL (Biological study)

(from latex of Euphorbia kamerunica)

L17 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1984:20456 HCAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER:

1984:20456 HC

TITLE:

The dermatitis-producing constituents of Euphorbia

hermentiana latex

AUTHOR(S):

Lin, Lee Juian; Marshall, Gary T.; Kinghorn, A.

Douglas

CORPORATE SOURCE:

Coll. Pharm., Univ. Illinois, Chicago, IL, 60612, USA

SOURCE:

Journal of Natural Products (1983), 46(5), 723-31

CODEN: JNPRDF; ISSN: 0163-3864

DOCUMENT TYPE:

LANGUAGE:

Journal English

GΙ

I, R^1 =Pr(CH:CH)3CO, R^2 =H, R^3 =CH2O2CCMe:CHMe, R^4 =OH II, R^1 =MeCH:CMeCO2, R^2 =Ac, R^3 =CH2OAc, R^4 =OAc III, R^1 =MeCH:CMeCO2, R^2 =H, R^3 =CH2OAc, R^4 =OAc IV, R^1 =MeCH:CMeCO2, R^2 =H, R^3 =Me, R^4 =OAc V, R^1 =MeCH:CMeCO2, R^2 =R 4 =H, R^3 =CH2OAc

AB Five ingenane derivs. 3-O-n-(deca-2,4,6-trienoyl)-16-O-[(Z)-2-methyl-2-butenoyl]-16-hydroxyingenol(I), 3-O-[(Z)-2-methyl-2-butenoyl]-5,16,20-O-triacetyl-16-hydroxyingenol(II), 3-O-[(Z)-2-methyl-2-butenoyl]-16,20-O-diacetyl-16-hydroxyingenol(III), 3-O-[(Z)-2-methyl-2-butenoyl]-20-O-acetylingenol(IV), and 3-O-[(Z)-2-methyl-2-butenoyl]-16-O-acetyl-20-deoxy-16-hydroxyingenol(V) were isolated with a new procedure that uses droplet counter-current chromatog., from a dermatitis-producing fraction of the latex of E. hermentiana. The structures of II, III, and V were established by the interpretation of their spectroscopic data and those of their hydrolytic and acetylated derivs.

IT 52557-27-4 82425-35-2 88262-74-2 88262-75-3 88262-77-5

RL: BIOL (Biological study)

(of Euphorbia hermentiana latex, dermatitis-producing)

RN 52557-27-4 HCAPLUS

CN 2,4,6-Decatrienoic acid, (1S,1aR,2S,5R,5aR,6S,8aS,9R,10aR)1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,7,9trimethyl-1-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester (9CI) (CA INDEX NAME)

PAGE 1-A

Me

Me

CH2-O-C

N-Pr-CH=CH-CH=CH-CH=CH-C-O

HO

$$CH_2$$
-OH

PAGE 1-B

RN 82425-35-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aS, 6S, 8aS, 9R, 10aR)-4[(acetyloxy)methyl]-1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-1, 1, 7, 9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

88262-74-2 HCAPLUS

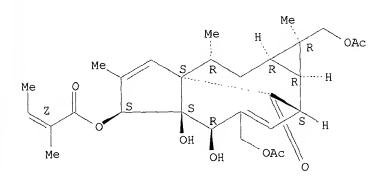
RN 88262-75-3 HCAPLUS

RN

2-Butenoic acid, 2-methyl-, 1,4-bis[(acetyloxy)methyl]1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,
[1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.
beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



RN 88262-77-5 HCAPLUS

IT 83966-49-8P 88262-78-6P 88262-79-7P 88262-81-1P 88262-82-2P 88262-84-4P 88262-85-5P 88262-86-6P 88262-88-8P 88262-90-2P 88262-91-3P 88262-92-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 83966-49-8 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl)methyl ester, [1aR-[1a.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)

RN 88262-78-6 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, [la,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-4-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-1-yl]methyl ester, [lR-[1.alpha.(Z),la.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 88262-79-7 HCAPLUS

2,4,6-Decatrienoic acid, [la,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,7,9-trimethyl-1-[[(2-methyl-1-oxo-2-butenyl)oxy]methyl]-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [lR-[1.alpha.(Z),la.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

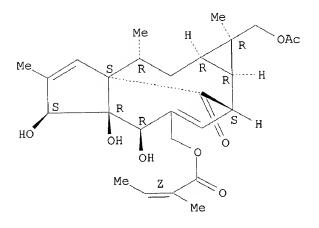
Absolute stereochemistry.

Double bond geometry as described by E or Z.

88262-81-1 HCAPLUS RN

2-Butenoic acid, 2-methyl-, [1-[(acetyloxy)methyl]-la,2,5,5a,6,9,10,10a-CN octahydro-5,5a,6-trihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha., la.beta., 2.alpha., 4(Z), 5.alpha., 5a.alpha., 6.alpha., 8a.beta., 9.beta., 10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.



88262-82-2 HCAPLUS RN 2-Butenoic acid, 2-methyl-, [1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-CN trihydroxy-1-(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha., la.beta., 2.alpha., 4(Z), 5.alpha., 5a.alpha., 6.alpha., 8a.beta., 9.beta., 10a.beta.]] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 88262-84-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, [5,6-bis(acetyloxy)-1-[(acetyloxy)methyl]1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester,
[1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,
9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 88262-85-5 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-4-[(acetyloxy)methyl]1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1-(hydroxymethyl)-1,7,9trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl
ester, [1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.b
eta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 88262-86-6 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR, 2S, 5R, 5aR, 6S, 8aS, 9R, 10aR)-5-(acetyloxy)-4[(acetyloxy)methyl]-1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5a-hydroxy-1, 1, 7, 9tetramethyl-11-oxo-1H-2, 8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 88262-88-8 HCAPLUS

2-Butenoic acid, 2-methyl-, [5,6-bis(acetyloxy)-1a,2,5,5a,6,9,10,10a-octahydro-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [laR-[la.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)

RN 88262-90-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 5-(acetyloxy)-1-[(acetyloxy)methyl]1a,2,5,5a,6,9,10,10a-octahydro-5a-hydroxy-1,4,7,9-tetramethyl-11-oxo-1H2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester,
[1R-[1.alpha.,1a.beta.,2.alpha.,5.alpha.,5a.alpha.,6.alpha.(Z),8a.beta.,9.
beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 88262-91-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, l-[(acetyloxy)methyl]-la,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester,
[1R-[1.alpha.,la.beta.,2.alpha.,5.alpha.(Z),5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 88262-92-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, la,2,5,5a,6,9,10,10a-octahydro-5a,6-dihydroxy-1-(hydroxymethyl)-1,4,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-5-yl ester,
[1R-[1.alpha.,la.beta.,2.alpha.,5.alpha.(Z),5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

11-1 (Plant Biochemistry)

Section cross-reference(s): 1, 30, 63

STEuphorbia ingenane deriv; dermatitis Euphorbia ingenol deriv; diterpene Euphorbia ingenol deriv

ΙT Dermatitis

(from ingenane derivs. of Euphorbia hermentiana latex)

IT Euphorbia trigona

(ingenane derivs. of, dermatitis-producing)

ITDiterpenes and Diterpenoids

RL: BIOL (Biological study)

(of Euphorbia hermentiana latex, dermatitis-producing)

IT83036-62-8

RL: BIOL (Biological study)

(acyl rearrangement of with acium hydroxide)

IΤ 52557-27-4 82425-35-2 88262-74-2

88262-75-3 88262-77-5

RL: BIOL (Biological study)

(of Euphorbia hermentiana latex, dermatitis-producing)

IT 30220-45-2P 52557-30-9P **83966-49-8P 88262-78-6P**

88262-79-7P 88262-81-1P 88262-82-2P

88262-83-3P 88262-84-4P 88262-85-5P

88262-86-6P 88262-88-8P 88262-90-2P

88262-91-3P 88262-92-4P 88262-93-5P 88262-95-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

L17 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1983:122775 HCAPLUS

DOCUMENT NUMBER:

98:122775

TITLE:

SOURCE:

Three new ingenane derivatives from the latex of

Euphorbia canariensis L

AUTHOR(S):

Lin, Lee Juian; Kinghorn, A. Douglas

CORPORATE SOURCE:

Coll. Pharm., Univ. Illinois, Chicago, IL, 60612, USA

Journal of Agricultural and Food Chemistry (1983),

31(2), 396-400

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GΙ

AB Three new ingenane esters, 3-O-acetyl-16-O-benzoyl-20-O-[(Z)-2-methyl-2-butenoyl]-16-hydroxyingenol (I), 3-O-[(Z)-2-methyl-2-butenoyl]-16-O-benzoyl-16-hydroxyingenol, and 3-O-acetyl-20-O-[(Z)-2-methyl-2-butenoyl]ingenol, were isolated from the latex of E. canariensis by using droplet countercurrent chromatog. The structures of these compds. were established through the interpretation of spectroscopic data. The compds. are known skin irritants.

Ι

IT 83966-45-4 83966-46-5 83983-93-1 RL: BIOL (Biological study)

(of Euphorbia canariensis latex)

RN 83966-45-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, [6-(acetyloxy)-1-[(benzoyloxy)methyl]1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,7,9-trimethyl-11-oxo-1H2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester,
[1S-[1.alpha.,1a.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.
alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)

RN 83966-46-5 HCAPLUS

2-Butenoic acid, 2-methyl-, [6-(acetyloxy)-la,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,7,9-tetramethyl-ll-oxo-lH-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester,

[laR-[la.alpha.,2.beta.,4(Z),5.beta.,5a.beta.,6.beta.,8a.alpha.,9.alpha.,10a.alpha.]]- (9CI) (CA INDEX NAME)

RN 83983-93-1 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4(hydroxymethyl)-1,7,9-trimethyl-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 83966-48-7P 83966-49-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)
RN 83966-48-7 HCAPLUS

2-Butenoic acid, 2-methyl-, [1-[(benzoyloxy)methyl]-1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,7,9-trimethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl]methyl ester, [1R-[1.alpha.,1a.beta.,2.alpha.,4(Z),5.alpha.,5a.alpha.,6.alpha.,8a.beta.,9.beta.,10a.beta.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

RN 83966-49-8 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (la,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-4-yl)methyl ester,

[laR-[la.alpha., 2.beta., 4(Z), 5.beta., 5a.beta., 6.beta., 8a.alpha., 9.alpha., 1 Oa.alpha.]]- (9CI) (CA INDEX NAME)

CC 11-1 (Plant Biochemistry)

STEuphorbia diterpene ester ingenane; ingenane latex Euphorbia

ΙŢ Euphorbia canariensis

(diterpene esters of latex of)

IT Diterpenes and Diterpenoids

RL: BIOL (Biological study)

(esters, of Euphorbia canariensis)

IT 83966-45-4 83966-46-5 83983-93-1

RL: BIOL (Biological study)

(of Euphorbia canariensis latex)

83966-47-6P **83966-48-7P** TT 30220-45-2P 52557-30-9P

83966-49-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

L17 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2002 ACS 1980:617929 HCAPLUS ACCESSION NUMBER:

93:217929 DOCUMENT NUMBER:

TITLE: Constituents of Egyptian Euphorbiaceae. IX. Irritant

and cytotoxic ingenane esters from Euphorbia paralias

AUTHOR(S): Sayed, M. D.; Riszk, A.; Hammouda, F. M.; El-Missiry,

M. M.; Williamson, E. M.; Evans, F. J.

Pharm. Sci. Lab., Natl. Res. Cent., Cairo, Egypt CORPORATE SOURCE:

SOURCE: Experientia (1980), 36(10), 1206-7

CODEN: EXPEAM; ISSN: 0014-4754

DOCUMENT TYPE: Journal English LANGUAGE:

The irritant and cytotoxic constituents of the latex of E. paralias were sepd. from the hydrocarbon fraction by solvent partition. Three new ingenane esters were identified from the toxic ether fraction. The major compd. was 3-angelyl-20-deoxyingenol and the 2 minor compds. were 3-hexanoyl-20-deoxyingenol and 3-angelylingenol. These compds. were of a similar potency to podophyllin in the inhibition of thymidine-3H uptake by TLX/5 mouse lymphoma cells. In addn., the compds. produced a persistent erythema of the mouse ear in sub-microgram doses.

TΤ 75567-37-2 75567-38-3

RL: BIOL (Biological study)

(from Euphorbia paralias, cytotoxic and irritant activities of)

75567-37-2 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)-1a, 2, 5, 5a, 6, 9, 10, 10a-octahydro-5, 5a-dihydroxy-4-(hydroxymethyl)-1, 1, 7, 9tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6yl ester, (2Z) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.

RN 75567-38-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aR,2S,5R,5aS,6S,8aS,9R,10aR)1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-1,1,4,7,9-pentamethyl-1l-oxo1H-2,8a-methanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester, (2Z)(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (~). Double bond geometry as shown.

CC 11-1 (Plant Biochemistry)

Section cross-reference(s): 1

ST ingenane ester Euphorbia

IT Diterpenes and Diterpenoids RL: BIOL (Biological study)

(from Euphorbia paralias, cytotoxic and irritant activities of)

IT Euphorbia paralias

(ingenane esters from, cytotoxic and irritant activity of)

IT Cytotoxic agents

(ingenane esters, from Euphorbia paralias)

IT **75567-37-2 75567-38-3** 75567-39-4

RL: BIOL (Biological study)

(from Euphorbia paralias, cytotoxic and irritant activities of)

IT 30220-46-3P 54706-99-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and acetylation of)

IT 30220-45-2P 54707-00-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

L17 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1974:146346 HCAPLUS

DOCUMENT NUMBER: 80:146346

TITLE: New diterpenoid irritants from Euphorbia ingens

AUTHOR(S): Opferkuch, H. J.; Hecker, E.

TATE 09/888,997

CORPORATE SOURCE:

Inst. Biochem., Dtsch. Krebsforschungszent.,

Heidelberg, Ger.

SOURCE:

Tetrahedron Lett. (1974), (3), 261-4

CODEN: TELEAY

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI For d

For diagram(s), see printed CA Issue.

AB The irritants I, II, and III, and the non-irritants IV and the 3,7,12-triacetate-8-nicotinate of ingol, were isolated from the latex of Euphorbia ingens. On the mouse ear, III showed an irritant dose 50 of 0.02 .mu.g/ear and II a dose of 0.004 .mu./ear.

IT 52557-27-4

RL: BOC (Biological occurrence); BIOL (Biological study); OCCU

(Occurrence)

(of Euphorbia ingens)

RN 52557-27-4 HCAPLUS

CN 2,4,6-Decatrienoic acid, (1S,1aR,2S,5R,5aR,6S,8aS,9R,10aR)1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,7,9trimethyl-1-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-11-oxo-1H-2,8amethanocyclopenta[a]cyclopropa[e]cyclodecen-6-yl ester (9CI) (CA INDEX
NAME)

PAGE 1-B

CC 30-20 (Terpenoids)

Section cross-reference(s): 11

ST Euphorbia terpenoid irritant

IT Skin, toxic chemical and physical damage (for Euphorbia ingens diterpenoids)

IT Diterpenoids

RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)

(of Euphorbia ingens)

IT Euphorbia ingens

(terpenoid irritants of)

IT 39071-33-5 51906-00-4 52557-26-3 **52557-27-4** 52557-28-5 RL: BOC (Biological occurrence); BIOL (Biological study); OCCU (Occurrence)

(of Euphorbia ingens)

IT 52557-29-6P 52557-30-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

=> d ibib abs hitstr 1-16

T22 ANSWER 1 OF 16 HCAPLUS / COPYRIGHT 2002 ACS ACCESSION NUMBER: 2001:439629 HCAPLUS

DOCUMENT NUMBER:

136:256788

TITLE:

Triterpenoid acids from Schisandra propinqua with cytotoxic effect on rat luteal cells and human

decidual cells in vitro

AUTHOR(S):

SOURCE:

Chen, Y.-G.; Qin, G.-W.; Cao, L.; Leng, Y.; Xie, Y.-Y.

CORPORATE SOURCE:

Department of Chemistry, Yunnan Normal University, Kunming, Yunnan, 650092, Peop. Rep. China

Fitoterapia (2001), 72(4), 435-437

CODEN: FTRPAE; ISSN: 0367-326X

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

Journal English

LANGUAGE: English

AB Three triterpenoid acids, nigranoic acid (1), manwuweizic acid (2), schisandronic acid (3), and other four compds. were isolated from the stems of Schisandra propinqua. Compds. 1 and 2 showed significant cytotoxic effect against human decidual cells and rat luteal cells in

vitro.

IT 39111-07-4P, Nigranoic acid 55511-14-3P, Schisandronic acid

RL: PAC (Pharmacological activity); PUR (Purification or

recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(triterpenoid acids from Schisandra propinqua with cytotoxic effect on rat luteal cells and human decidual cells in vitro)

RN 39111-07-4 HCAPLUS

CN 1H-Cyclopenta[a]cyclopropa[e]naphthalene-3a(4H)-propanoic acid, 7-[(1R,4Z)-5-carboxy-1-methyl-4-hexenyl]decahydro-6a,9a-dimethyl-3-(1-methylethenyl)-, (3S,3aR,4aS,6aR,7R,9aS,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me
$$\frac{CH_2}{S}$$
 $\frac{Me}{S}$ $\frac{S}{R}$ $\frac{CO_2H}{Me}$ $\frac{R}{Me}$ \frac

RN 55511-14-3 HCAPLUS

CN 9,19-Cyclolanost-24-en-26-oic acid, 3-oxo-, (24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2002 ACS 2000:456898 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

133:88533

TITLE: Compositions obtained from Mangifera indica L. INVENTOR(S): Nunez Selles, Alberto Julio; Paez Betancourt,

> Eleuterio; Amaro Gonzalez, Daniel; Acosta Esquijarosa, Jhoany; Aguero Aguero, Juan; Capote Hernandez, Raul; Garciga Hernandez, Maria Rosa; Morales Lacarrere, Ivan Gaston; Garcia Pulpeiro, Oscar; Garrido Garrido,

Gabino; Martinez Sanchez, Gregorio; Morales, Miguel Centro de Quimica Farmaceutica, Cuba

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

Spanish LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ENT	NO.		KI	ND	DATE			А	PPLI	CATI	ON I	NO.	DATE	
						~			_						
WO 2000038699			A1		2000	0706		WO 1999-CU7					19991229		
	T.T.	73. 5. 7	DD	~ 7	CAT	T D	TNI	TD	MV	דזמ	CD	7,11	TIC	7.7 N.T	

W: AU, BR, CA, CN, ID, IN, JP, MX, RU, SD, UA, US, VN
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG CU 1998-203 A 19981229 PRIORITY APPLN. INFO.:

The present invention relates essentially to the pharmaceutical, food and cosmetic industries and in particular to the prepn. of formulations of active principles which are derived from bark of the plant Mangifera indica, among which are the polyphenols, the terpenoids, the steroids, the fatty acids and microelements which have antioxidant, antiinflammatory, analgesic and antispasmodic properties, thereby conferring to said formulations high value as dietary supplements for the improvement of the quality of life of patients suffering from degenerative diseases, as well as for anti-aging treatment and for consumption by healthy persons.

13878-90-5, Mangiferonic acid ΙT

RL: BUU (Biological use, unclassified); FFD (Food or feed use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(compns. obtained from Mangifera indica for health food and drugs and cosmetics)

RN 13878-90-5 HCAPLUS CN 9,19-Cyclolanost-24-en-26-oic acid, 3-oxo-, (24E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1999:567080 HCAPLUS

DOCUMENT NUMBER: 131:317356

TITLE: Activity of triterpenoid glycosides from the root bark

of Mussaenda macrophylla against two oral pathogens

AUTHOR(S): Kim, Nam-Cheol; Desjardins, Anne E.; Wu, Christine D.;

Kinghorn, A. Douglas

CORPORATE SOURCE: Program for Collaborative Research in the

Pharmaceutical Sciences and Department of Medicinal Chemistry and Pharmacognosy College of Pharmacy, University of Illinois, Chicago, IL, 60612, USA

SOURCE: Journal of Natural Products (1999), 62(10), 1379-1384

CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

Four new triterpenoid glycosides were isolated from the root bark of Mussaenda macrophylla. Their structures were detd. as 3-O-.beta.-D-glucopyranosyl-28-O-.alpha.-L-rhamnopyranosyl-16.alpha.hydroxy-23-deoxyprotobassic acid (1), 28-O-.beta.-D-glucopyranosyl-16.alpha.-hydroxy-23-deoxyprotobassic acid (2), 3-0-.beta.-Dglucopyranosyl-28-0-.alpha.-L-rhamnopyranosyl-16.alpha.-hydroxyprotobassic acid (3), and 3-0-{[.beta.-D-glucopyranosyl-(1.fwdarw.6)]-0-.alpha.-Lrhamnopyranosyl-(1.fwdarw.2)-O-.beta.-D-glucopyranosyl-(1.fwdarw.2)}-O-.beta.-D-glucopyranosyl-(1.fwdarw.3)-O-.beta.-D-glucopyranosyl-cycloarta-22,24-dien-27-oic acid (mussaendoside W, 4). Four known triterpenoids [3-O-acetyloleanolic acid (5), 3-O-acetyldaturadiol (6), rotundic acid (7), and 16.alpha.-hydroxyprotobassic acid (8)] were also isolated. The structures of 1-4 were detd. by several spectroscopic techniques including 2D NMR methods. Compds. 1-6 showed inhibitory activity against a periodontopathic bacterium, Porphyromonas gingivalis, but were inactive against the cariogenic organism, Streptococcus mutans.

IT 248912-10-9P, Mussaendoside W
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
 (activity of triterpenoid glycosides from the root bark of Mussaenda)

macrophylla against two oral pathogens)

RN 248912-10-9 HCAPLUS
9,19-Cyclolanosta-22,24-dien-26-oic acid, 3-[(0-6-deoxy-.alpha.-Lmannopyranosyl-(1.fwdarw.2)-0-[.beta.-D-glucopyranosyl-(1.fwdarw.6)]-0.beta.-D-glucopyranosyl-(1.fwdarw.2)-0-[.beta.-D-glucopyranosyl(1.fwdarw.3)]-.beta.-D-glucopyranosyl)oxy]-, (3.beta.,22E,24E)- (9CI)
INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

PAGE 1-B

PAGE 2-A

REFERENCE COUNT:

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1999:532419 HCAPLUS

25

DOCUMENT NUMBER: 131:283964

TITLE: Resveratrol tetramers from Vatica diospyroides

AUTHOR(S): Seo, Eun-Kyoung; Chai, Heebyung; Constant, Howard L.;

Santisuk, Thawatchai; Reutrakul, Vichai; Beecher, Christopher W. W.; Farnsworth, Norman R.; Cordell, Geoffrey A.; Pezzuto, John M.; Kinghorn, A. Douglas

CORPORATE SOURCE: Program for Collaborative Research in the

Pharmaceutical Sciences and Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy

University of Illinois at Chicago, Chicago, IL, 60612,

USA

SOURCE: Journal of Organic Chemistry (1999), 64(19), 6976-6983

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB Vatdiospyroidol (I), a novel cytotoxic resveratrol tetramer, was isolated from the stems of Vatica diospyroides Sym. (Dipterocarpaceae) by bioassay-guided fractionation monitored with a human oral epidermoid carcinoma (KB) cell line. Another novel resveratrol tetramer, vaticaphenol A (II), was obtained as a noncytotoxic constituent, along with the known compds., bergenin, betulin, betulinic acid, mangiferonic acid, and (E)-resveratrol 3-O-.beta.-D-glucopyranoside. The structures of compds. I and II were elucidated by spectral anal., including 1D and 2D NMR expts., and by mol. modeling.

NMR expts., and by mol. modeling. IT 13878-90-5, Mangiferonic acid

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(from Vatica diospyroides)

RN 13878-90-5 HCAPLUS

CN 9,19-Cyclolanost-24-en-26-oic acid, 3-oxo-, (24E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

REFERENCE COUNT:

43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1999:4251 HCAPLUS

DOCUMENT NUMBER:

130:34353

TITLE:

Dietary cancer risk conditional cancerogens in produce of livestock fed on species of spurge (Euphorbiaceae).

Part 1. Skin irritant and tumor-promoting

ingenane-type diterpene esters in E. peplus, one of several herbaceous Euphorbia species contaminating fodder of livestock. [Erratum to document cited in

CA129:312034]

AUTHOR(S):

Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamby;

Gotta, Hubert; Hecker, Erich

CORPORATE SOURCE:

Laboratory Organic Chemistry, National Research

Center, Cairo, Egypt

SOURCE:

Journal of Cancer Research and Clinical Oncology

(1998), 124(6), 351

CODEN: JCROD7; ISSN: 0171-5216

PUBLISHER:

Springer-Verlag

Journal

DOCUMENT TYPE: LANGUAGE: English

AB On page 135, in Table 2, the words "Low" in the last column should read "Medium"; the complete column is reprinted.

214771-74-1P IT

RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(skin irritant and tumor-promoting ingenane-type diterpene esters in Euphorbia (Erratum))

RN 214771-74-1 HCAPLUS

2-Butenoic acid, 2-methyl-, (laS, 2R, 2aR, 3aR, 5R, 5aS, 8S, 8aS, 9S, 9aR)-CN 1a, 2, 2a, 3a, 4, 5, 8, 8a, 9, 9a-decahydro-8a, 9-dihydroxy-3, 3, 5, 7, 9a-pentamethyl-10-oxo-3H-2,5a-methanocyclopenta[4,5]cyclopropa[8,9]cyclodec[1,2-b]oxiren-8-yl ester, (2Z)- (9CI) (CA INDEX NAME)

L22 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:577094 HCAPLUS

DOCUMENT NUMBER: 129:312034

TITLE: Dietary cancer risk conditional cancerogens in produce

of livestock fed on species of spurge (Euphorbiaceae).

Part 1. Skin irritant and tumor-promoting

ingenane-type diterpene esters in E. peplus, one of several herbaceous Euphorbia species contaminating

fodder of livestock

AUTHOR(S): Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamdy;

Gotta, Hubert; Hecker, Erich

CORPORATE SOURCE: Laboratory Organic Chemistry, National Research

Center, Cairo, Egypt

SOURCE: Journal of Cancer Research and Clinical Oncology

(1998), 124(3/4), 131-140

CODEN: JCROD7; ISSN: 0171-5216

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal LANGUAGE: English

Several herbaceous plants of the genus Euphorbia, widespread as weeds and contaminants of livestock fodder, were identified botanically and exts. of their aerial parts were tested for irritancy on the mouse ear. As compared to a std. probe of croton oil, the exts. of E. peplus, E. nubica, and E. helioscopia displayed irritancy. The most active ext. (that from E. peplus) was investigated by a fractionation procedure monitored by the mouse ear assay, and 5 molecularly uniform irritant E. factors Pe1-Pe5 were identified as diterpene ester-type toxins. Together these factors comprise at least 11 ppm in the aerial parts. They were characterized individually to carry the diterpene parent alcs. ingenol, 20-deoxyingenol, and 20-deoxyingenol-6.alpha.,7.alpha.-epoxide. The irritancy of the aerial plant parts was caused mainly by the E. factors Pel and Pe2 together. Upon chronic administration of these irritants and hyperplasiogens as principal cancerogenic risk factors in the mouse skin initiation/promotion bioassay, Pel and Pe2 were established as tumor promoters.

IT 214771-74-1P

RL: ADV (Adverse effect, including toxicity); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(skin irritant and **tumor**-promoting ingenane-type diterpene esters in Euphorbia)

RN 214771-74-1 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1aS, 2R, 2aR, 3aR, 5R, 5aS, 8S, 8aS, 9S, 9aR) - 1a, 2, 2a, 3a, 4, 5, 8, 8a, 9, 9a-decahydro-8a, 9-dihydroxy-3, 3, 5, 7, 9a-pentamethyl-10-oxo-3H-2, 5a-methanocyclopenta[4,5]cyclopropa[8,9]cyclodec[1,2-b]oxiren-

8-yl ester, (2Z)- (9CI) (CA INDEX NAME)

L22 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:443284 HCAPLUS

DOCUMENT NUMBER: 127:70830

TITLE: Isolation of triterpene acids from Kadsura japonica as

anti-androgen agents

INVENTOR(S): Hayashi, Katsuhiro; Suzuki, Tatsuhiko; Oishi, Seiko;

Yagi, Kunio; Koda, Mayumi; Kakita, Shingo; Yokoo,

Yoshiharu; Honda, Shinkichi; Tadano, Toshio

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan; Kyowa Medex Co.,

Ltd.; Oyo Seikagaku Kenkyusho K. K.

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09151196 JP 3260918	A2 B2	19970610 20020225	JP 1993-171671	19930712

OTHER SOURCE(S): MARPAT 127:70830

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB The title compds. (I; X = O, single bond; R = H, OH) are isolated by extn. from Kadsura japonica using alcs. I are useful as anti-androgen agents for prevention and treatment of hair diseases such as male hair loss, prostatic hypertrophy, prostatic cancer, and related diseases. The title compd. (II) showed IC50 of 4.3 X 10-8 M against androgen receptor binding activity. Formulation contg. II is presented.
- 1T 190836-57-8P 190836-60-3P 190836-64-7P
 RL: BAC (Biological activity or effector, except adverse); BSU
 (Biological study, unclassified); PUR (Purification or recovery); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(isolation of triterpene acids from Kadsura japonica as anti-androgen agents)

RN 190836-57-8 HCAPLUS

CN .beta.-D-Glucopyranose, 1-[(2Z,6R)-6-[(5aR,6aS,8aR,9R,11aS,11bS,13aR)-

tetradecahydro-1,1,8a,11a-tetramethyl-3-oxo-3H,6H-cyclopenta[5,6]cyclopropa[1,8a]naphth[2,1-c]oxepin-8-yl]-2-methyl-2-heptenoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 190836-60-3 HCAPLUS

.beta.-D-Glucopyranose, 1-[(2Z,6R)-6-[(5aR,6aS,8aR,9R,11aS,11bS,13R,13aS)-tetradecahydro-13-hydroxy-1,1,8a,11a-tetramethyl-3-oxo-3H,6H-cyclopenta[5,6]cyclopropa[1,8a]naphth[2,1-c]oxepin-8-yl]-2-methyl-2-heptenoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+). Double bond geometry as shown.

RN 190836-64-7 HCAPLUS CN 9,19-Cyclolanost-24-en-26-oic acid, 6-hydroxy-3-oxo-, .beta.-D-glucopyranosyl ester, (6.beta.,24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-). Double bond geometry as shown.

L22 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:618612 HCAPLUS

DOCUMENT NUMBER: 125:257163

TITLE: Antiandrogenic triterpenes and their extraction from

Kadsura japonica

INVENTOR(S): Hayashi, Katsuhiro; Suzuki, Tatsuhiko; Ooishi,

Shigeko; Yagi, Kunio; Koda, Mayumi; Kakita, Shingo; Yokoo, Yoshiharu; Pponda, Shinkichi; Tadano, Toshio

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Kk, Japan; Kyowa Medex Co Ltd; Oyo

Seikagaku Kenkyusho

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08193094	A2	19960730	JP 1995-3025	19950112

OTHER SOURCE(S): MARPAT 125:257163

AB Novel antiandrogenic triterpenes and their extn. from K. japonica are claimed. Two compds. extd. from K. japonica are purified and characterized by spectrochem. and other methods. For dosage form prepns., 2 mg of the antiandrogenic triterpene was dissolved in 100 mL ethanol, mixed with 10 mg dextrin, and dried. Capsules were formulated contg. the powder 3, lactose 121, corn starch 50 and hydroxypropyl cellulose 16 mg.

IT 182123-23-5P 182123-26-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(novel antiandrogenic triterpenes and their extn. from Kadsura japonica) $\label{eq:control}$

RN 182123-23-5 HCAPLUS

CN 9,19-Cyclolanost-24-en-26-oic acid, 6-hydroxy-, 6-O-(4-carboxy-3-hydroxy-3-methyl-1-oxobutyl)-.beta.-D-glucopyranosyl ester, (6.beta.,24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

__CO2H

182123-26-8 HCAPLUS RN

.beta.-D-Glucopyranose, 6-O-(4-carboxy-3-hydroxy-3-methyl-1-oxobutyl)-, CN 1-[(2Z,6R)-6-[(5aR,6aS,8aR,9R,11aS,11bS,13R,13aS)-tetradecahydro-13hydroxy-1,1,8a,11a-tetramethyl-3-oxo-3H,6H-cyclopenta[5,6]cyclopropa[1,8a] naphth[2,1-c]oxepin-8-yl]-2-methyl-2-heptenoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

PAGE 1-A

PAGE 1-B

__CO2H

L22 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1996:437039 HCAPLUS

DOCUMENT NUMBER:

125:132052

TITLE:

Analgesic and anti-inflammatory activity of

tetracyclic triterpenoids isolated from Pistacia

integerrima galls

AUTHOR(S):

SOURCE:

Ansari, S. H.; Ali, M.

CORPORATE SOURCE:

Fac. Pharmacy, Jamia Hamdard, New Delhi, 110062, India

Fitoterapia (1996), 67(2), 103-105

CODEN: FTRPAE; ISSN: 0367-326X

PUBLISHER:

Inverni della Beffa SpA

DOCUMENT TYPE:

Journal

LANGUAGE: English

The analgesic and anti-inflammatory activity of six tetracyclic triterpenoids, pistacigerrimones A, B, C, D, E and F, isolated from the AΒ galls of P. integerrima was studied. Pistacigerrimones C and D gave highly significantly results.

ΙT 158372-26-0, Pistacigerrimone F

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(analgesic and anti-inflammatory activity of tetracyclic

triterpenoids isolated from Pistacia integerrima galls)

RN 158372-26-0 HCAPLUS

ON 9,19-Cyclolanosta-1,7,24-trien-26-oic acid, 3-oxo-, (24Z)- (9CI) (CAINDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

L22 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:265316 HCAPLUS

DOCUMENT NUMBER: 124:284381

TITLE: Nigranoic Acid, a Triterpenoid from Schisandra

sphaerandra That Inhibits HIV-1 Reverse Transcriptase AUTHOR(S): Sun, Han-dong; Qiu, Sheng-xiang; Lin, Long-ze; Wang,

Zong-yu; Lin, Zhong-wen; Pengsuparp, Thitima; Pezzuto,

John M.; Fong, Harry H. S.; Cordell, Geoffrey A.;

Farnsworth, Norman R.

CORPORATE SOURCE: Kunming Institute of Botany, Chinese Academy of

Sciences, Kunming, 650204, Peop. Rep. China

SOURCE: Journal of Natural Products (1996), 59(5), 525-7

CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB An A ring-secocycloartene triterpenoid, nigranoic acid (3,4-secocycloarta-4(28),24-(Z)-diene-3,26-dioic acid), was isolated from the stems of Schisandra sphaerandra, a Chinese traditional medicinal plant. Its structure elucidation and unambiguous NMR spectral assignment were achieved by the combination of 1D- and 2D-NMR techniques with the aid of computer modeling. Nigranoic acid showed activity in several anti-HIV reverse transcriptase and polymerase assays.

IT 39111-07-4, Nigranoic Acid

RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(nigranoic acid triterpenoid from Schisandra sphaerandra inhibitor of HIV-1 Reverse Transcriptase)

RN 39111-07-4 HCAPLUS

CN 1H-Cyclopenta[a]cyclopropa[e]naphthalene-3a(4H)~propanoic acid, 7-[(1R,4Z)-5-carboxy-1-methyl-4-hexenyl]decahydro-6a,9a-dimethyl-3-(1-methylethenyl)-, (3S,3aR,4aS,6aR,7R,9aS,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L22 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:531979 HCAPLUS

DOCUMENT NUMBER: 115:131979

TITLE: Isolation and structures of schisanlactone E and

changnanic acid

AUTHOR(S): Liu, Jiasen; Huang, Meifen

CORPORATE SOURCE: Shanghai Inst. Mater. Med., Acad. Sin., Shanghai,

200031, Peop. Rep. China

SOURCE: Huaxue Xuebao (1991), 49(5), 502-6

CODEN: HHHPA4; ISSN: 0567-7351

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

- AB Two new triterpenoid compds., schisanlactone E (I) and changnanic acid (II), along with three known compds., schisanlactone B (III), meso-dihydroguaiaretic acid and .beta.-sitosterol, were isolated from the root bark of Kadsura longipedunculata Finet. et Gagnep. indigenous to the Lin-An district in Zhejiang province of China. Their structures were elucidated by spectroscopic studies. In an anticancer screening I and II show significant inhibition of leukemia p-388 cells in vitro (IC50 1 .mu.g/mL and 10 .mu.g/mL resp.).
- IT 136040-44-3

RL: BIOL (Biological study)

(of Kadsura longipedunculata, isolation, mol. structure and neoplasm inhibiting activity of)

RN 136040-44-3 HCAPLUS

CN 3H-Cyclopenta[a]cyclopropa[e]naphthalene-3a(4H)-propanoic acid, 7-[(1R,4Z)-5-carboxy-1-methyl-4-hexenyl]-5,6,6a,7,8,9,9a,9b-octahydro-6a,9a-dimethyl-3-(1-methylethenyl)-, (3S,3aR,4aS,6aR,7R,9aS,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me
$$\frac{1}{2}$$
 $\frac{1}{2}$ \frac

L22 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1991:489129 HCAPLUS

DOCUMENT NUMBER: 115:89129

Isolation and structures of schisantherin J and TITLE:

schisanlactone F

Liu, Jiasen; Pan, Yanping AUTHOR(S):

Shanghai Inst. Mater. Med., Chin. Acad. Sci., CORPORATE SOURCE:

> Shanghai, 200031, Peop. Rep. China Huaxue Xuebao (1991), 49(3), 308-12 CODEN: HHHPA4; ISSN: 0567-7351

DOCUMENT TYPE: Journal LANGUAGE: Chinese

GT

SOURCE:

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB One new lignan, schisantherin J(I) and one new triterpenoid, schisanlactone F (II) were isolated along with four known compds., schisanlactone A, schizandronic acid, epianwuweizic acid and di-Me deangeloyl schisantherin F, from the seed of Kadsura longipeduaculata Finet. et Gagnep. Their structures including abs. configurations were elucidated by spectroscopic studies and chem. conversions. In anticancer screening, II shows a significant inhibition of leukemia P-388 cells in vitro (ED50 5 .mu.g/mL).

55511-14-3, Schisandronic acid IT

RL: PROC (Process)

(isolation of, from Kadsura longipedunculata)

55511-14-3 HCAPLUS RN

9,19-Cyclolanost-24-en-26-oic acid, 3-oxo-, (24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown:

L22 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:489752 HCAPLUS

DOCUMENT NUMBER: 109:89752

TITLE: Studies on the constituents of Schisandraceae plants

in Shennongjia District. I. Constituents of Schisandra

propinqua Hook. F. et Thoms. var. sinensis Oliv

AUTHOR(S): Liu, Jiasen; Ma, Yuting; Huang, Meifen

CORPORATE SOURCE: Shanghai Inst. Mater. Med., Acad. Sin., Shanghai,

Peop. Rep. China

SOURCE: Huaxue Xuebao (1988), 46(4), 345-8

Ι

CODEN: HHHPA4; ISSN: 0567-7351

DOCUMENT TYPE: Journal LANGUAGE: Chinese

OTHER SOURCE(S): CASREACT 109:89752

GΙ

AB Six compds. were isolated from the stems and roots of S. propinqua var. sinensis. One is a new lignan named epienshicine (I), m.p. 163-164.degree., [.alpha.]Dll.5 -18.2.degree. (CHCl3), which was shown to be 1-oxy-2R,3S-dimethyl-4R-(3-methoxy-4-hydroxyphenyl)-6,7-methylenedioxytetralin by means of spectral anal. and chem. transformation into (+)-galcatin. The remaining five compds. were identified as enshicine, isoschisandrolic acid (II), deoxyschizandrin, .beta.-sitosterol, and stearic acid, in which II is isolated from the natural resources for the first time. I shows activity against leukemia P-388 in vitro.

IT 55511-17-6

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)

(of Schisandra propinqua)

RN 55511-17-6 HCAPLUS

CN 9,19-Cyclolanost-24-en-26-oic acid, 3-hydroxy-, (3.beta.,24Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

L22 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:507324 HCAPLUS

DOCUMENT NUMBER: 101:107324

TITLE: On the active principles of the Euphorbiaceae, IX.

Ingenane type diterpene esters from five Euphorbia

species

AUTHOR(S): Gotta, H.; Adolf, W.; Opferkuch, H. J.; Hecker, E.

CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent.,

Heidelberg, D-6900, Fed. Rep. Ger.

SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische

Chemie, Organische Chemie (1984), 39B(5), 683-94

CODEN: ZNBAD2; ISSN: 0340-5087

DOCUMENT TYPE: Journal LANGUAGE: English

AB Investigation of E. antiquorum, E. helioscopia, E. palustris, E. peplus, and E. quadrialata for irritant and tumor-promoting constituents afforded several new ingenane diterpene esters derived from the parent alcs. ingenol and 20-deoxyingenol and from the hitherto unknown 20-deoxy-16-hydroxyingenol and 20-deoxy-13,16-dihydroxyingenol. The irritant activities of the natural compds. are reported, together with some aspects on structure activity relationships.

IT 87980-68-5

RL: BIOL (Biological study) (from Euphorbia species)

RN 87980-68-5 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 6,6a,7a,8,9,12,12a,12b-octahydro-12a-hydroxy-2,2,7,7,9,11-hexamethyl-13-oxo-7H-6,9a-methano-4H-cyclopenta[9,10]cyclopropa[5,6]cyclodeca[1,2-d]-1,3-dioxin-12-yl ester,[6R-[6.alpha.,6a.alpha.,7a.alpha.,9.alpha.,9a.alpha.,12.beta.(Z),12a.beta.,12b.alpha.]]- (9CI) (CA INDEX NAME)

IT 91413-77-3P

RN 91413-77-3 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, 1a,2,3,9,12,12a-hexahydro-1,1,3,5,7,7,10-heptamethyl-13-oxo-5aH-3a,12-methano-1H-cyclopropa[5',6']cyclodeca[1',2':1,5]cyclopenta[1,2-d][1,3]dioxol-9-yl ester, [1aR-[1a.alpha.,3.alpha.,3a.alpha.,5a.alpha.,8aR*,9.beta.(Z),12.beta.,12a.alpha.]]- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L22 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:12496 HCAPLUS

DOCUMENT NUMBER: 100:12496

TITLE: 3-0-Angeloylingenol, the toxic and skin irritant

factor from latex of Euphorbia antiquorum L.

(Euphorbiaceae) and from a derived Thai purgative and

anthelimintic (vermifuge) drug

AUTHOR(S): Adolf, W.; Chanai, S.; Hecker, E.

CORPORATE SOURCE: Inst. Biochem., Dtsch. Krebsforschungszent.,

Heidelberg, D-6900, Fed. Rep. Ger.

SOURCE: Journal of the Science Society of Thailand (1983),

9(2), 81-8

CODEN: VKSTDB; ISSN: 0303-8122

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

From a latex of E. antiquorum, as well as from the purgative and AΒ anthelmintic (vermifuge) Thai drug yang Sa-Lad-Dai (dried, powd. latex), the highly skin irritant and toxic Euphorbia factor Anl 3-O-angeloylingenol (I) [75567-37-2] was isolated by combination of countercurrent distributions and chromatog. Because of the acute toxicity of I and of the possible risk of cocarcinogenesis by tumor promotion, utilization of drugs made up from dried or fresh latex as practiced in Thailand in purgatives and vermifuges should be abandoned.

IT87980-68-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

87980-68-5 HCAPLUS

2-Butenoic acid, 2-methyl-, 6,6a,7a,8,9,12,12a,12b-octahydro-12a-hydroxy-CN 2,2,7,7,9,11-hexamethyl-13-oxo-7H-6,9a-methano-4Hcyclopenta[9,10]cyclopropa[5,6]cyclodeca[1,2-d]-1,3-dioxin-12-yl ester, [6R-[6.alpha.,6a.alpha.,7a.alpha.,9.alpha.,9a.alpha.,12.beta.(Z),12a.beta.,12b.alpha.]]- (9CI) (CA INDEX NAME)

L22 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1983:12688 HCAPLUS

DOCUMENT NUMBER:

98:12688

TITLE:

On the active principles of the spurge family (Euphorbiaceae). IV. Skin irritant and tumor promoting diterpene esters from Euphorbia ingens E.

Mey

AUTHOR(S):

Opferkuch, H. J.; Hecker, E.

CORPORATE SOURCE:

Inst. Biochem., Dtsch. Krebsforschungszent.,

Heidelberg, D-6900/1, Fed. Rep. Ger.

SOURCE:

Journal of Cancer Research and Clinical Oncology

(1982), 103(3), 255-68

CODEN: JCROD7; ISSN: 0171-5216

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GΙ

Me O
$$CH_2R^5$$

Me OR2

 CH_2R^4
 CH_2OR^4

Ι

The irritant and tumor-promoting principles of the latex of AΒ Euphorbia ingens were isolated together with several nonirritant compds. The Euphorbia factor Il [52557-26-3], I5 [52557-27-4], and I6 [52557-28-5] are esters of ingenane-type polyfunctional diterpene alcs. (I). Euphorbia factor Il is characterized as the 3-hexadecanoate of I and Euphorbia factor I6 as the 3-deca-2.4.6-trienoic acid ester of I. Euphorbia factor I5 is the 16-angelate-3-deca-2.4.6-trienoate of 16-hydroxyingenol. Nonirritant diterpenes of the latex are I2 [39071-33-5], the ingenol-20-hexadecanoate - an isomer of Euphorbia factor I1 - and I4, the 3.7.12-triacetate-8-nicotinate of the macrocyclic lathyrane-type polyfunctional diterpene alc. ingol. The diterpene alcs. ingenol and 16-hydroxyingenol are inactive as irritants and tumor promoters of mouse skin. Compared to croton oil factor A1, the Euphorbia factor Il exhibits .apprx.1/10 of the irritant and tumor -promoting activity in mouse skin. Il shows no reasonable tumorigenic activity. Compared with Il, Euphorbia factors I5 and 16 are more potent irritants and less potent tumor promoters.

ΙT 83919-97-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and dealkylation of)

RN 83919-97-5 HCAPLUS

2,4,6-Decatrienoic acid, 6,6a,7,7a,8,9,12a,12b-octahydro-12a-hydroxy-CN 2,2,7,9,11-pentamethyl-7-[[(2-methyl-1-oxo-2-butenyl)oxy]methyl]-13-oxo-12H-6, 9a-methano-4H-cyclopenta[9,10]cyclopropa[5,6]cyclodeca[1,2-d]-1,3dioxin-12-yl ester, [6R-(6.alpha.,6a.alpha.,7.alpha.,7a.alpha.,9.alpha.,9a .alpha.,12.beta.,12a.beta.,12b.alpha.)]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

= CH- Me

=> d ibib abs

SOURCE:

L26 ANSWER 1 OF 1 TOXCENTER COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:975 TOXCENTER COPYRIGHT: Copyright 2002 ASHP

DOCUMENT NUMBER: 30-12301

TITLE: Skin irritant principle from Euphorbia griseola

AUTHOR(S): Gundidza, M.; Sorg, B.; Hecker, E.

CORPORATE SOURCE: Germany Cancer Res. Ctr., Inst. of Biochem., Im Neuenheimer Feld 280, D-6900 Heidelberg, Germany

International Pharmacy Journal (Netherlands), (Jan-Feb

1993) Vol. 7, pp. 19-21. 13 Refs CODEN: IPHJEN. ISSN: 1010-0423.

DOCUMENT TYPE: Journal FILE SEGMENT: IPA

OTHER SOURCE: IPA 93:3196
LANGUAGE: English

SUMMARY LANGUAGE: French; German; Spanish ENTRY DATE: Entered STN: 20011116

Last Updated on STN: 20011116

AB Euphorbia factor EG1, a diterpene of the

ingenane-type parent alcohol with angelic acid as the acid substituent, was isolated from Euphorbia griseola and its irritant activity was studied using the mouse ear test. The skin irritant activity of the compound 24 h after administration was found to be 0.348 n mole/ear.

Ellen Katz Neumann

L23 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS

RN 157807-48-2 REGISTRY

CN Euphorbia factor EG1 (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1H-2,8a-Methanocyclopenta[a]cyclopropa[e]cyclodecene, euphorbia factor EG1 deriv.

OTHER NAMES:

CN 1H-2,8a-Methanocyclopenta[a]cyclopropa[e]cyclodecen-11-one,
1a,2,5,5a,6,9,10,10a-octahydro-5,5a,6-trihydroxy-4-(hydroxymethyl)-1,1,
7,9-tetramethyl-, mono[(Z)-2-methyl-2-butenoate],
(1aR,2S,5R,5aR,6S,8aS,9R,10aR)-

CN Ingenol monoangelate

FS STEREOSEARCH

MF C25 H34 O6

CI IDS

SR American Society of Hospital Pharmacists

Ring System Data

Elemental	Į	Elemental	S	ize	of	Ri	ng	System	n	Ring			RII	
Analysis	1	Sequence	1th	e R:	ings	1	For	cmula	Ide	entif	ier	10cc	curr	ence
EA	1	ES	1	SZ		İ	F	RF	1	RID			Cour	nt
==========	=+:	*=***=*=*=	+==:	-==	-===	+==	===		-+===	====	===-	⊦= = =	====	
C3-C5-C7-C7	7 0	C3-C5-C7-C7	13-	5-7-	-7	IC1	5		1280	9.1.	1	1	in	CM
	1		1			1			1			1		

CM 1

CRN 30220-46-3 CMF C20 H28 O5

Absolute stereochemistry.

CM 2

CRN 565-63-9 CMF C5 H8 O2

Double bond geometry as shown.

=> d ibib abs

L32 ANSWER 1 OF 2 TOXCENTER COPYRIGHT 2002 ACS ACCESSION NUMBER: 1975:71877 TOXCENTER COPYRIGHT: Copyright 2002 ACS DOCUMENT NUMBER: CA08221133804E TITLE: Diterpene esters from Euphorbium and their irritant and cocarcinogenic activity Hergenhahn, M.; Kusumoto, S.; Hecker, E. AUTHOR(S): CORPORATE SOURCE: Dtsch. Krebsforschungszent., Inst. Biochem., Heidelberg. SOURCE: Experientia, (1974) Vol. 30, No. 12, pp. 1438-40. CODEN: EXPEAM. DOCUMENT TYPE: Journal FILE SEGMENT: CAPLUS OTHER SOURCE: CAPLUS 1975:133804 LANGUAGE: English ENTRY DATE L32 ? 34 came from AB Diterr resini e ear for 12-deo Some text searching nmole/ 90-71-5], and 0. ate (III) [54662 tumor 1 - still nothing really with 0. mixt., $0.1 \, .mu$ 42.3, for using this stuff to treat cancer resp.

=> d ibib abs 2

resp.

L32 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1975:133804 CAPLUS

DOCUMENT NUMBER: 82:133804

TITLE: Diterpene esters from Euphorbium and their irritant

and cocarcinogenic activity

AUTHOR(S): Hergenhahn, M.; Kusumoto, S.; Hecker, E. CORPORATE SOURCE: Dtsch. Krebsforschungszent., Inst. Biochem.,

Heidelberg, Ger.

SOURCE: Experientia (1974), 30(12), 1438-40

CODEN: EXPEAM

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

Diterpene esters were obtained from air-dried latex of Euphorbia resinifera. The 3-hr irritant dose 50 (ID50) was 0.18 nmole/mouse ear for 12-deoxyphorbol-13-angelate-20-acetate (I) [25090-72-6], 0.024 nmole/ear for 12-deoxyphorbol-13-isobutyrate-20-acetate (II) [25090-71-5], and 0.0027 nmole/ear for 12-deoxyphorbol-13-phenylacetate-20-acetate (III) [54662-30-5]. Two ingol esters were not irritant. Percentage of tumor bearers among surviving mice, treated topically with 0.2 .mu.mole I, 0.2 II, 0.1 III, and 0.1 ingenol 3-acylate mixt., twice weekly for 12 weeks, following tumor initiation by 0.1 .mu.mole 7,12-dimethylbenz[a]anthracene, was 11.1, 0, 7.4, and 42.3,

=> d ibib abs 1-10

L34 ANSWER 1 OF 10 MEDLINE ?

ACCESSION NUMBER: 2000280699 MEDLINE

20280699 PubMed ID: 10821064 DOCUMENT NUMBER: Diterpenoids from Euphorbia peplus. TITLE: Hohmann J; Evanics F; Berta L; Bartok T AUTHOR: PLANTA MEDICA, (2000 Apr) 66 (3) 291-4. SOURCE:

Journal code: 0066751. ISSN: 0032-0943. GERMANY: Germany, Federal Republic of

PUB. COUNTRY: DOCUMENT TYPE: Letter LANGUAGE: English

Priority Journals FILE SEGMENT:

ENTRY MONTH: 200006

ENTRY DATE: Entered STN: 20000706

Last Updated on STN: 20000706 Entered Medline: 20000626

AR From a pro-inflammatory active extract of Euphorbia peplus, two new diterpene polyesters based on the pepluane and jatrophane skeletons were isolated, together with four known ingenane and jatrophane diterpenes. The structures were determined on the basis of extensive NMR studies. Ingenol 3-angelate, which was obtained for the first time from this plant, is an irritant toxin with high activity.

L34 ANSWER 2 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 1

ACCESSION NUMBER: 2000:146716 TOXCENTER Copyright 2002 ACS COPYRIGHT:

DOCUMENT NUMBER: CA13307086701D Diterpenoids from Euphorbia peplus TITLE:

Hohmann, Judit; Evanics, Ferenc; Berta, Laszlo; Bartok, AUTHOR(S):

CORPORATE SOURCE: Department of Pharmacognosy, Albert Szent-Gyorgyi Medical

University, Szeged, 6701, Hung...

Planta Medica, (2000) Vol. 66, No. 3, pp. 291-294. CODEN: PLMEAA. ISSN: 0032-0943. SOURCE:

HUNGARY COUNTRY: DOCUMENT TYPE: Journal CAPLUS FILE SEGMENT:

OTHER SOURCE: CAPLUS 2000:310802

LANGUAGE: English

ENTRY DATE: Entered STN: 20011116

Last Updated on STN: 20020326

From a pro-inflammatory active ext. of Euphorbia peplus, two new diterpene polyesters I and II based on the pepluane and jatrophane skeletons were isolated, together with four known ingenane and jatrophane diterpenes. The structures were detd. on the basis of extensive NMR studies. Ingenol 3-angelate, which was obtained for the first time from this plant, is an irritant toxin with high activity.

L34 ANSWER 3 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 2

ACCESSION NUMBER: 1998:89050 TOXCENTER Copyright 2002 BIOSIS COPYRIGHT: DOCUMENT NUMBER: PREV199800394066

TITLE: Dietary cancer risk from conditional

cancerogens in produce of livestock fed on species of spurge (Euphorbiaceae). III. Milk of lactating goats fed on the skin irritant herb Euphorbia peplus is polluted

by tumor promoters of the ingenane

diterpene ester type

Zayed, Salah M. A. D.; Farghaly, Madiha; Taha, Hamdy; AUTHOR(S):

Gminski, Richard; Hecker, Erich (1)

(1) Deutsches Krebsforschungszentrum, Div. S0109, Res. CORPORATE SOURCE:

Program 3, Risk Factors Cancer Cancer Prevention, In

Neuenheimer Feld 280, D-69120 Heidelberg Germany

Journal of Cancer Research and Clinical Oncology, (June,

1998) Vol. 124, No. 6, pp. 301-306.

ISSN: 0171-5216.

Article DOCUMENT TYPE: FILE SEGMENT: BIOSIS

SOURCE:

OTHER SOURCE: BIOSIS 1998:394066

LANGUAGE: English

Entered STN: 20011116 ENTRY DATE:

Last Updated on STN: 20011116

Special procedures were developed to investigate poisonous milk of lactating goats fed experimentally on aerial parts of the herb Euphorbia peplus L. In extracts of the milk, weakly irritant in the mouse-ear assay, three diterpene ester toxins were detected by techniques of high-performance liquid chromatography. They are of the ingenane structural type: Euphorbia factor Pel (ingenol 20-acetate 3-

angelate), Euphorbia factor Pe2 (20-deoxyingenol 3angelate) and Euphorbia factor Pe4 (20-deoxyingenol -6alpha, 7alpha-epoxide 3-angelate). From goats milk collected 15 days after cessation of the experimental feeding period, extracts were completely free of diterpene ester toxins. The toxins polluting the milk are identical to diterpene ester entities occurring in the aerial parts of E. peplus. Of these, Euphorbia factors Pel and Pe2 are known as promoters of tumors of mouse skin. Apart from the toxic Euphorbia factors, the non-toxic parent alcohol ingenol was also detected in the milk. It is absent in the plant, and may have been generated metabolically from a certain portion of the toxic diterpene esters picked up by the goats from their fodder. The results presented here provide, for the first time, data for a novel interpretation of the locally high incidence of esophageal cancer observed in certain areas in the Caspian littoral of Iran, associated with a greater consumption of goat's

L34 ANSWER 4 OF 10 NAPRALERT COPYRIGHT (C) 2002 BD. TRUSTEES, U. IL.

ACCESSION NUMBER: 1998:6172 NAPRALERT

DOCUMENT NUMBER: J16371

(and sheep's) milk.

DIETARY CANCER RISK CONDITIONAL CANCEROGENS TITLE:

IN PRODUCE OF LIVESTOCK FED ON SPECIES OF SPURGE (EUPHORBIACEAE). I. SKIN IRRITANT AND TUMOR -PROMOTING INGENANE-TYPE DITERPENE ESTER IN

E.PEPLUS, ONE OF SEVERAL HERBACEOUS EUPHORBIA SPECIES

CONTAMINATING FODDER OF LIVESTOCK

ZAYED S M A D; FARGHALY M; TAHA H; GOTTA H; HECKER E AUTHOR:

CORPORATE SOURCE: LAB ORG CHEM, NATL RES CENT, CAIRO EGYPT

J CANCER RES CLIN ONCOL (1998) 124 (3/4) p. 131-140. SOURCE:

DOCUMENT TYPE: (Research paper)

LANGUAGE: ENGLISH 4068 CHARACTER COUNT:

AUTHOR(S):

L34 ANSWER 5 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 3

ACCESSION NUMBER: 1985:140316 TOXCENTER

COPYRIGHT: Copyright 2002 ACS DOCUMENT NUMBER: CA10319157302T

Constituents of Egyptian Euphorbiaceae. Part 13. TITLE:

Biologically active diterpene esters from Euphorbia peplus Rizk, A. M.; Hammouda, F. M.; El-Missiry, M. M.; Radwan,

H. M.; Evans, F. J.

CORPORATE SOURCE: Pharm. Sci. Lab., Natl. Res. Cent., Cairo, Egypt.

SOURCE: Phytochemistry (Elsevier), (1985) Vol. 24, No. 7, pp.

1605-6.

CODEN: PYTCAS. ISSN: 0031-9422.

COUNTRY: EGYPT DOCUMENT TYPE: Journal

FILE SEGMENT: CAPLUS

OTHER SOURCE: CAPLUS 1985:557302 LANGUAGE: English

ENTRY DATE: Entered STN: 20011116

Last Updated on STN: 20021112

AB By means of partition and preparative TLC, 2 pro-inflammatory diterpene esters were isolated from E. peplus. These compds. were

identified as 20-deoxyingenol 3-0-angelate, which

exhibited an irritant dose (for 50% irritation) of 0.18 .mu.g on mouse

skin, and the new ester ingenol 20-0-octanoate (I), which

exhibited an irritant dose (for 50% irritation) of 1.0 .mu.g on mouse

skin.

L34 ANSWER 6 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 4

1983:65815 TOXCENTER

ACCESSION NUMBER: 1983:65815 TOXCENTER COPYRIGHT: Copyright 2002 BIOSIS

DOCUMENT NUMBER: BA75:15145

TITLE: INGENOL ESTERS FROM THE PRO INFLAMMATORY

FRACTION OF EUPHORBIA-KAMERUNICA

AUTHOR(S): ABO K A; EVANS F J

CORPORATE SOURCE: DEP. PHARMACOGNOSY, SCH. PHARMACY, UNIV. LONDON, 29-39,

BRUNSWICK SQUARE, LONDON, WC1N 1AX, UK.

SOURCE: PHYTOCHEMISTRY (OXF), (1982) 21 (3), 725-726

CODEN: PYTCAS. ISSN: 0031-9422.

FILE SEGMENT: BIOSIS

OTHER SOURCE: BIOSIS 1983:165145

LANGUAGE: English

ENTRY DATE: Entered STN: 20011116

Last Updated on STN: 20011116

AB A series of unstable mono- and diesters of the tetracyclic diterpene

ingenol were isolated from the proinflammatory ether-soluble
fraction of the latex of E. kamerunica. The esters were isolated by a
neutral process involving column chromatography and TLC. The monoesters
were identified by spectroscopic methods and hydrolysis reactions as

ingenol-3-decanoate, ingenol-3-dodecanoate,

ingenol-5-decandate, Ingenol-5-doctedandate,
ingenol-5-hexadienoate and ingenol-5-octenoate and the
diesters as 20-acetyl-ingenol-3-octenoate and 20-acetyl-

ingenol-3-angelate.

L34 ANSWER 7 OF 10 TOXCENTER COPYRIGHT 2002 ACS DUPLICATE 5

ACCESSION NUMBER: 1983:71571 TOXCENTER COPYRIGHT: Copyright 2002 BIOSIS

DOCUMENT NUMBER: BA75:58451

TITLE: THE ACTIVE PRINCIPLES OF THE SPURGE FAMILY EUPHORBIACEAE

4. SKIN IRRITANT AND TUMOR PROMOTING DI TERPENE

ESTERS FROM EUPHORBIA-INGENS

AUTHOR(S): OPFERKUCH H J; HECKER E

CORPORATE SOURCE: INST. BIOCHEM., DEUTSCHES KREBSFORSCHUNGSZENT., IM

NEUENHEIMER FELD 280, D-6900 HEIDELBERG 1, W. GER. J CANCER RES CLIN ONCOL, (1982) 103 (3), 255-268

CODEN: JCROD7. ISSN: 0171-5216.

FILE SEGMENT: BIOSIS

SOURCE:

OTHER SOURCE: BIOSIS 1983:208451

LANGUAGE: English

ENTRY DATE: Entered STN: 20011116

Last Updated on STN: 20011116

The irritant and tumor-promoting principles of the latex of E. ingens E. Mey were isolated with several nonirritant compounds. The Euphorbia factors I1, I5 and I6 are esters of ingenane-type polyfunctional diterpene alcohols. Euphorbia factor II is characterized as the 3-hexadecanoate of the polyfunctional parent alcohol ingenol and Euphorbia factor I6 as the 3-deca-2.4.6-trienoic acid ester of ingenol. Euphorbia factor I5 is the 16angelate-3-deca-2.4.6-trienoate of 16-hydroxyingenol. Nonirritant diterpenes of the latex are I2, the ingenol -2-hexadecanoate-an isomer of Euphorbia factor I1- and I4, the 3.7.12-triacetate-8-nicotinate of the macrocyclic lathyrane-type polyfunctional diterpene alcohol ingol. The diterpene alcohols ingenol and 16-hydroxyingenol are inactive as irritants and tumor promoters of mouse skin. Compared to croton oil factor A1 (TPA), the Euphorbia factor I1 exhibits about 1/10 of the irritant and tumor-promoting activity in mouse skin Il shows no reasonable tumorigenic activity. Compared with I1, Euphorbia factors I5 and I6 are more potent irritants and less potent tumor

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ACCESSION NUMBER: 6235562 BABS

TITLE: Diterpenoids from Euphorbia peplus

AUTHOR(S): Hohmann, Judit; Evanics, Ferenc; Berta, Laszlo;

Bartok, Tibor

SOURCE: Planta Med. (2000), 66(3), 291 - 294

CODEN: PLMEAA

DOCUMENT TYPE: Journal LANGUAGE: English SUMMARY LANGUAGE: English

AN 6235562 BABS

promoters.

AB From a pro-inflammatory active extract of Euphorbia peplus, two new diterpene polyesters based on the pepluane and jatrophane skeletons were isolated, together with four known ingenane and jatrophane diterpenes. The structures were determined on the basis of extensive NMR studies. Ingenol 3-angelate, which was obtained for the first time from this plant, is an irritant toxin with high activity.

L34 ANSWER 9 OF 10 BABS COPYRIGHT 2002 BEILSTEIN CDS MDLI

ACCESSION NUMBER: 5865227 BABS

TITLE: BIOLOGICALLY ACTIVE DITERPENE ESTERS FROM EUPHORBIA

PEPLUS

AUTHOR(S): Rizk, A. M.; Hammouda, F. M.; El-Missiry, M. M.;

Radwan, H. M.; Evans, F. J.

SOURCE: Phytochemistry (1985), 24(7), 1605-1606

CODEN: PYTCAS

DOCUMENT TYPE: Journal LANGUAGE: English SUMMARY LANGUAGE: English

AN 5865227 BABS

L34 ANSWER 10 OF 10 BABS COPYRIGHT 2002 BEILSTEIN CDS MDLI

ACCESSION NUMBER: 5828746 BABS

TITLE: INGENOL ESTERS FROM THE PRO-

INFLAMMATORY FRACTION OF EUPHORBIA KAMERUNICA

AUTHOR(S): Abo, Kio A.; Evans, Fred J.

SOURCE: Phytochemistry (1982), 21(3), 725-726

CODEN: PYTCAS

DOCUMENT TYPE: Journal LANGUAGE: English SUMMARY LANGUAGE: English

and 20-acetyl-ingenol-3-angelate.

AN 5828746 BABS

AB A series of unstable mono- and di-esters of the tetracyclic diterpene ingenol were isolated from the pro-inflammatory ether-soluble fraction of the latex of Euphorbia kamerunica. The esters were isolated by a neutral process involving column and thin-layer chromatography. The monoesters were identified by spectroscopic methods and hydrolysis reactions as ingenol-3-decanoate, ingenol

-3-dodecanoate, ingenol-5-hexadienoate and ingenol

-5-octenoate and the diesters as 20-acetyl-ingenol-3-octenoate